This journal is (c) The Royal Society of Chemistry 2010

Electronic Supplementary Information

Direct Oxidative Coupling of Benzenes with Acrylonitriles to Cinnamonitriles Catalyzed by $Pd(OAc)_2$/HPMoV/O_2 System

Yasushi Obora,* Yoshihisa Okabe, and Yasutaka Ishii*

Department of Chemistry and Materials Engineering, Faculty of Chemistry, Materials and Bioengineering, High Technology Research Center,and ORDIST Kansai University, Suita, Osaka 564-8680, Japan

Table of Contents

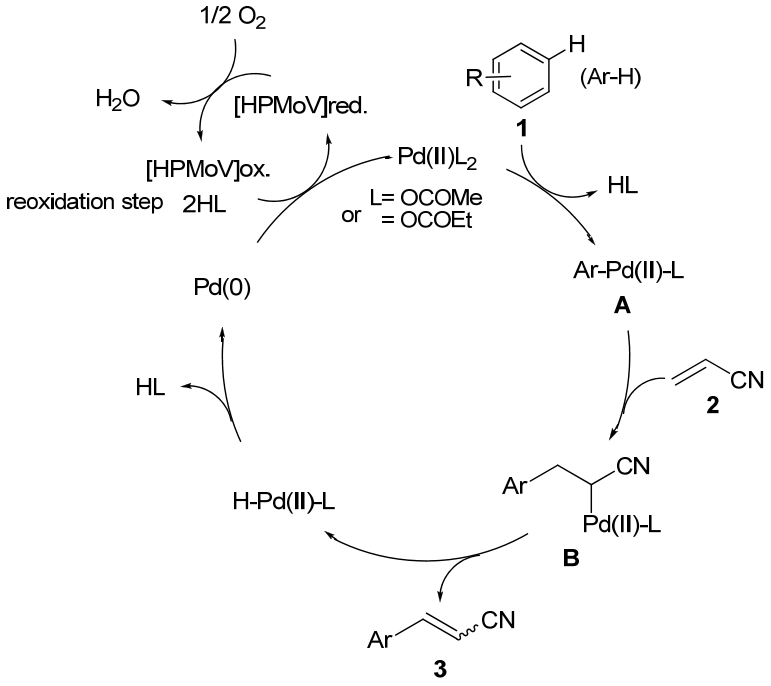


Figure S1 A plausible reaction path for the oxidative coupling of benzenes (**1**) with acrylonitriles (**2**) by $Pd(OAc)_2$/HPMoV/O_2 system.

Table S2. Full data to show all *E/Z* ratio in Table 2 in the manuscript.

Entry	Ar-H	Yield			Ratio of **3**				Yield
		Total(**3**+**4**)	**3**		ortho (*E*: *Z*)	meta (*E*: *Z*)	para (*E*: *Z*)		
1	Benzene	68[47]	**3a**	66[47]	*E*: Z = 75:25			**4a**	2
2	Toluene	58 [47]	**3b**	51[43]	23 (47:53)	29 (98:2)	48 (89:11)	**4b**	7[4]
3	Toluene	73	**3b**	66	23 (72:28)	38(73:27)	39 (49:51)	**4b**	7
4	Toluene	69	**3b**	59	22 (73:27)	38 (70:30)	40(50:50)	**4b**	10
5	Anisole	80[67]	**3c**	47[43]	22 (86: 14)	15 (67:33)	63 (42:58)	**4c**	33[24]
6	Chlorobenzene	29[28]	**3d**	29[28]	36 (67: 33)	27 (68:32)	37 (76:24)	**4d**	nd
7	p-xylene	46[37]	**3e**	46[37]	*E*: *Z* = 78:22			**4e**	trace

Table S3. Full data to show all *E/Z* ratio in Table 3 in the manuscript.

Entry	Ar-H	Yield	Ratio of **5**		
		5	ortho (*E*: *Z*)	meta (*E*: *Z*)	para (*E*: *Z*)
1	Benzene	**5a** 49[42]	*E*: *Z* = 32:68		
2	Toluene	**5b** 53[53]	21 (37:63)	43 (41:59)	36 (65:35)
3	anisole	**5c** 63[58]	13 (57:43)	23(16:84)	64 (33:67)
4	chlorobenzene	**5d** 51[47]	35 (74:26)	30 (62:38)	35(56:44)
7	p-xylene	**5e** 49[43]	*E*: *Z* = 32:68		

Experimental Section

Compounds **3a**,[1a] **3b**,[1b] **3c**,[1c] **3d**,[1d] **3e**,[1e] **4a**,[1f] **4b**,[1g] **4c**,[1h] **5a**,[1i] **5b**,[1j] **5c**,[1k] and **5d**[1l] were known compounds reported previously. Heteropolyacids were prepared according to a literature procedure.[2] The yields of products were estimated by GC from the peak areas based on an internal standard technique. The determination of *E*/*Z* stereochemistry were carried out by ^{1}H NMR and DPFGSE-NOE (double pulse field gradient spin echo) method.[3]

Experimental Procedure

A typical reaction procedure for the preparation of cinnamonitrile (3a) (Table 1, entry 2): A solution of $Pd(OAc)_2$ (22.4 mg, 0.1 mmol), $H_4PMo_{11}VO_{40}{\cdot}20H_2O$ (46.0 mg, 0.02 mmol), NaOAc (8.2 mg, 0.1 mmol), acetylacetone (10 mg, 0.1 mmol), benzene (**1a**) (7.03 g, 90 mmol), and acrylonitile (**2a**) (79.6 mg, 1.5 mmol) in propionic acid (10 mL) was placed in a round-bottom flask (50 mL) equipped with a balloon filled with O_2, and the mixture was allowed to react under stirring at 90 °C for 5 h. GC analysis of the reaction mixture showed that cinnamonitrile (**3a**) and β-phenylcinnamonitrile (**4a**) was obtained in 78% and 11% yields, respectively. The products, **3a** and **4a,** were isolated by column chromatography (160-200 mesh silica gel, *n*-hexane/ethyl acetate = 19/1) in 74% (143 mg) and 8% (25 mg) yields, respectively.

5e: colorless liquid, δ_H (400 MHz; $CDCl_3$, Me_4Si) *E* isomer: 7.18-6.81 (m, 3H), 5.15 (s, 1H), 2.28 (s, 3H), 2.24 (s, 3H) and 2.17 (s, 3H), *Z* isomer: 7.18-6.81 (m, 3H), 5.41(s, 1H), 2.25 (s, 3H), 2.18 (s, 3H) and 2.11 (s, 3H); δ_C (100 MHz; $CDCl_3$, Me_4Si) *E* isomer: 163.6 (C), 140.2 (C), 138.6 (C), 135.5 (C), 130.6 (CH), 129.3 (CH), 127.5 (CH), 116.7 (CN), 98.8 (CH), 22.9 (CH_3), 20.8 (CH_3) and 18.6 (CH_3), *Z* isomer: 163.9 (C), 140.2 (C), 138.6 (C), 135.5 (C), 130.5 (CH), 129.4 (CH), 127.1 (CH), 116.7 (CN), 98.3 (CH), 25.6 (CH_3), 20.9 (CH_3) and 19.3 (CH_3); ν_{max}/cm^{-1} for *E*,*Z* mixture: 3016, 2975, 2924, 2869, 2219, 1735, 1609, 1498, 1440, 1377, 1176, 1044 and 815; *m/z* (EI): *E* isomer: 171.1053 (M^+. $C_{12}H_{13}N$ requires 171.1049), 156 (24%), 144

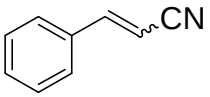
(36), 129 (100), 115 (16), 105 (6), 91(13), 77(15) and 63(9), *Z* isomer: 171.1052 (M^+. $C_{12}H_{13}N$ requires 171.1049), 156(24%), 144(32), 129(100), 115(18), 105(4), 91(15), 77(18) and 63(9).

References

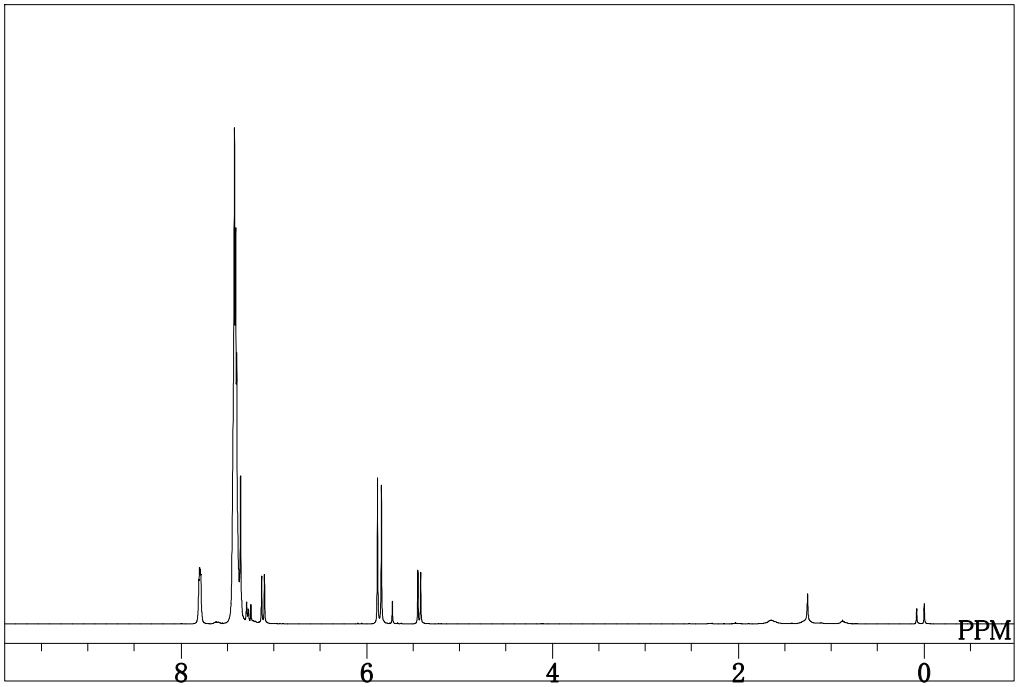
1 (*a*) J. D. Senra, L. F. B. Malta, A. L. F. Souza, L. C. S. Aguiar and O. A. C. Antunes, *Adv. Synth. Catal.,* 2008, **350**, 2551; (*b*) A. K. Gupta, C. H. Song and C. H. Oh, *Tetrahedron Lett.,* 2004, **45**, 4113; (*c*) H. B. Borate, D. K. Dumbre, R. D. Wakharkar and V. R. Choudhary, *J. Chem. Res.,* 2008, 495; (*d*) E. A. B. Kantchev, G.-R. Peh, C. Zhang and J. Y. Ying, *Org. Lett.,* 2008, **10**, 3949; (*e*) B. A. D'Sa, P. Kisanga and J. G. Verkade, *J. Org. Chem.,* 1988, **63**, 3961; (*f*) A. R. Gholap, V. Paul and K. V. Srinivasan, *Synth. Commun.,* 2008, **38**, 2967; (*g*) K. Shima, A. Sazaki, K. Nakabayashi and M. Yasuda, *Bull. Chem. Soc. Jpn.,* 1992, **65**, 1472; (*h*) M. Laubender and H. Werner, *Chem. Eur. J.,* 1999, **5**, 2937; (*i*) B. M. Choudary, M. L. Kantam, C. R. V. Reddy, B. Bharathi and F. Figueras, *J. Catal.* **2003**, 218, 191. (*j*) D. Lee, Y. Yang and J. Yun, *Synthesis*, 2007, 2233; (*k*) J. T. Gupton, D. Zembower and J. Miller, *Synth. Commun.,* 1988, **18**, 1891.

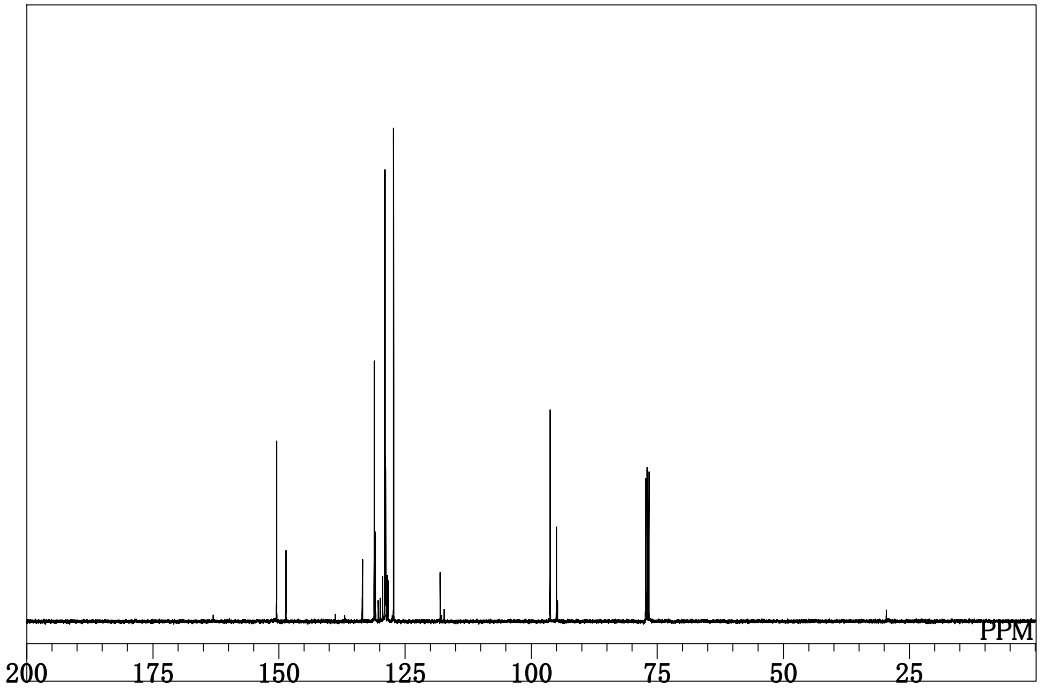
2. L. Pettersson, I. Andersson, J. H. Grate and A. Selling, *Inorg. Chem.,* 1994, **33**, 982.

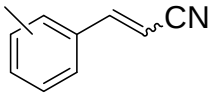
3. T.-L. Hwang and A. J. Shaka, *J. Magn. Reson. A* 1995, **112**, 275.



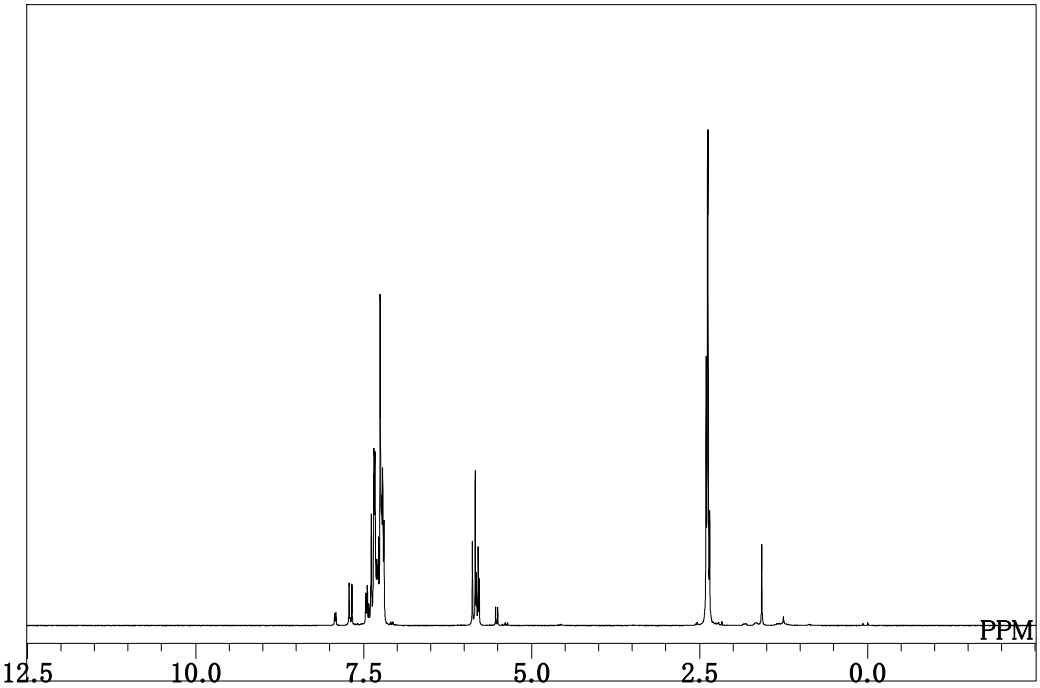
3a

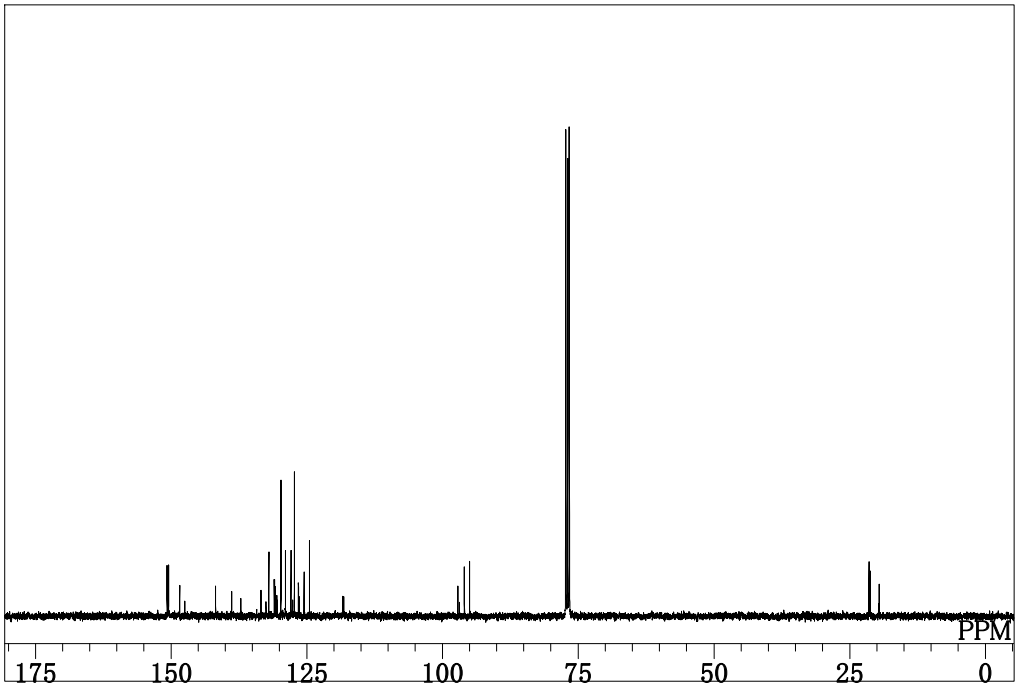


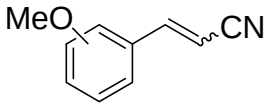




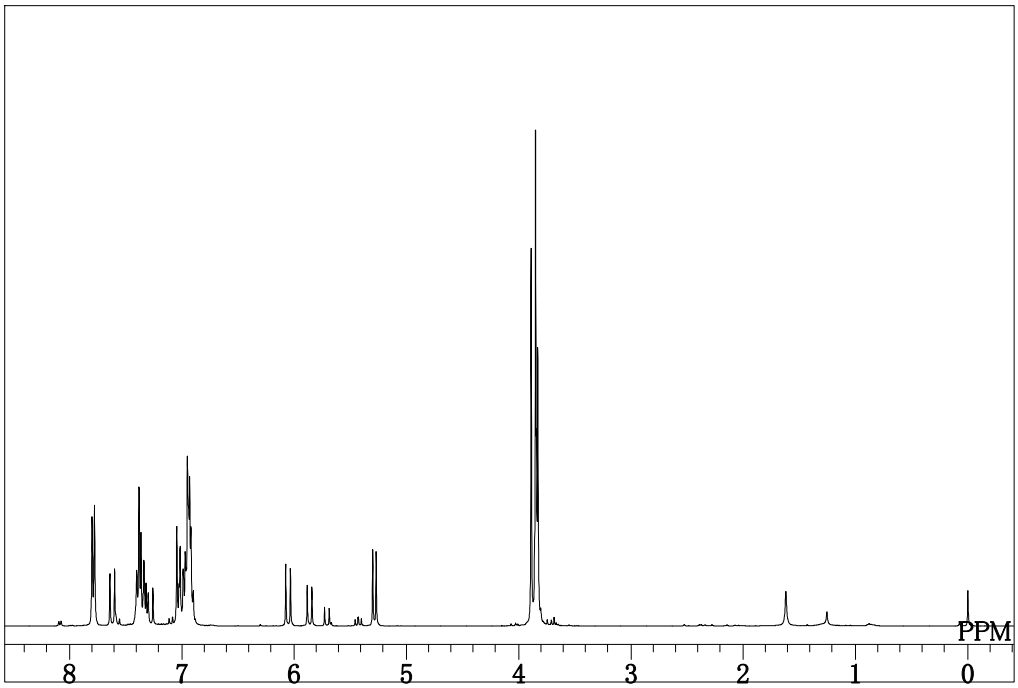
3b

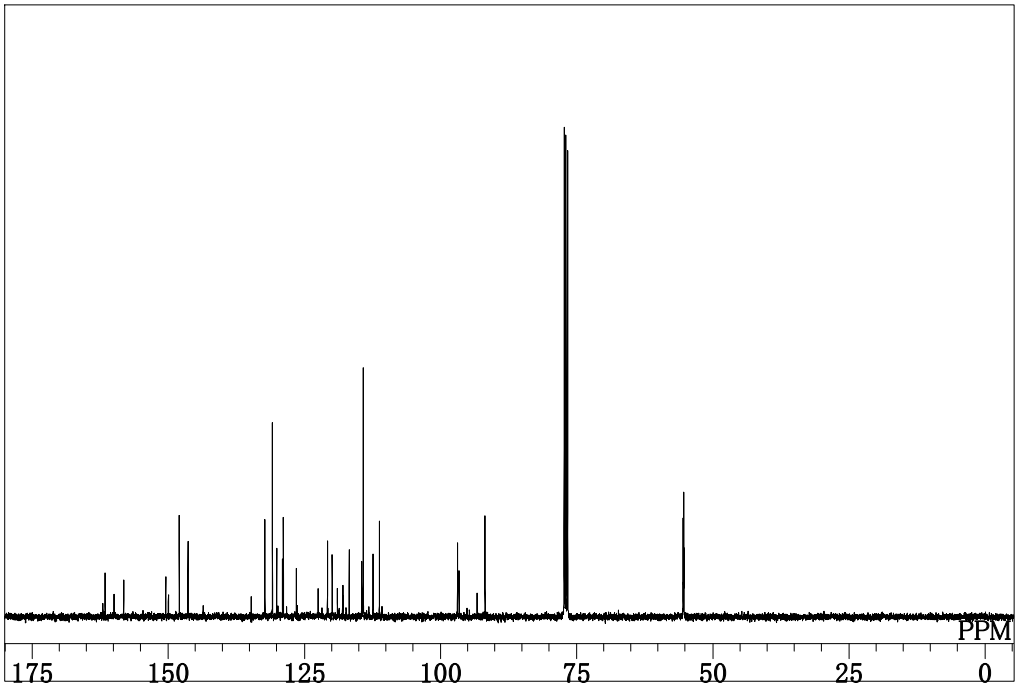


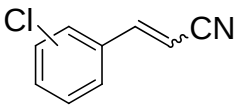




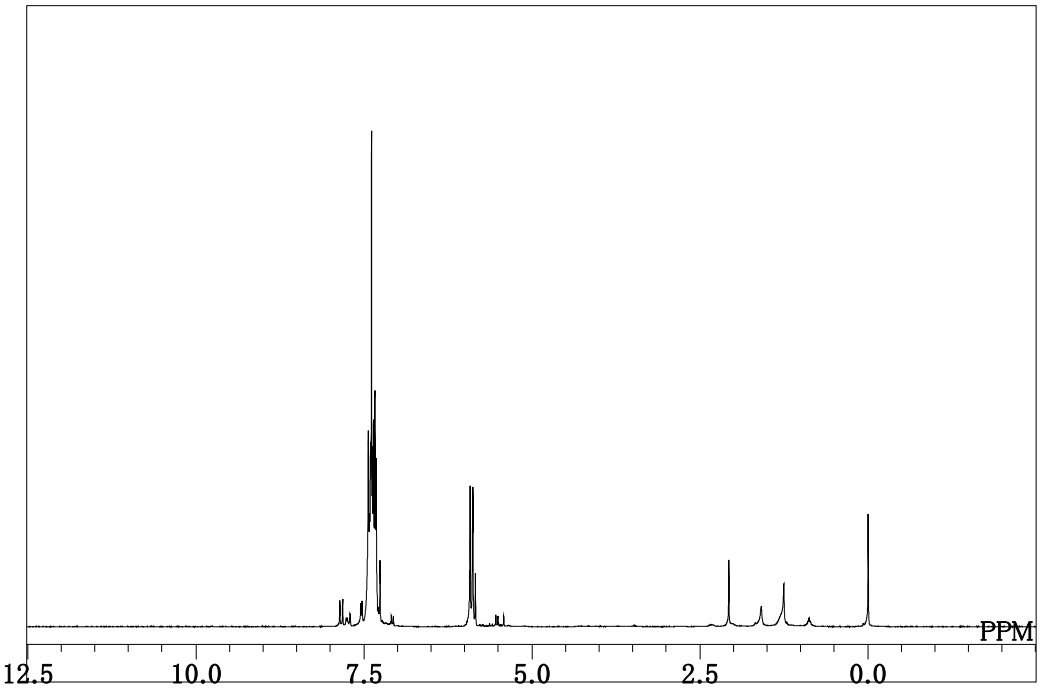
3c

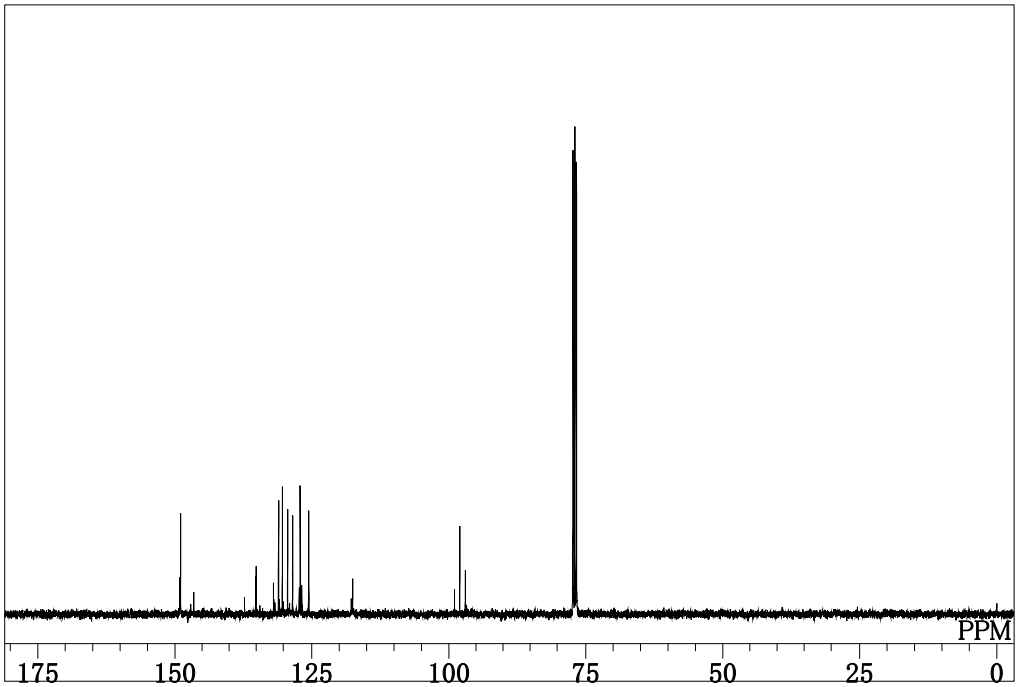


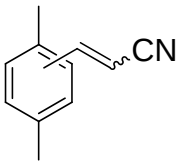




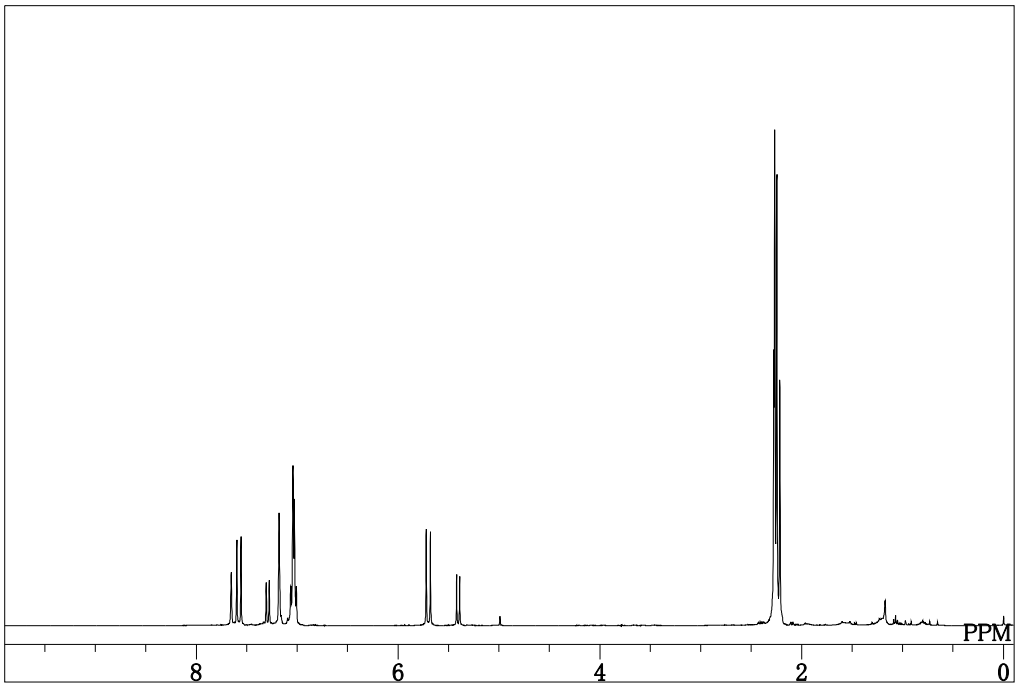
3d

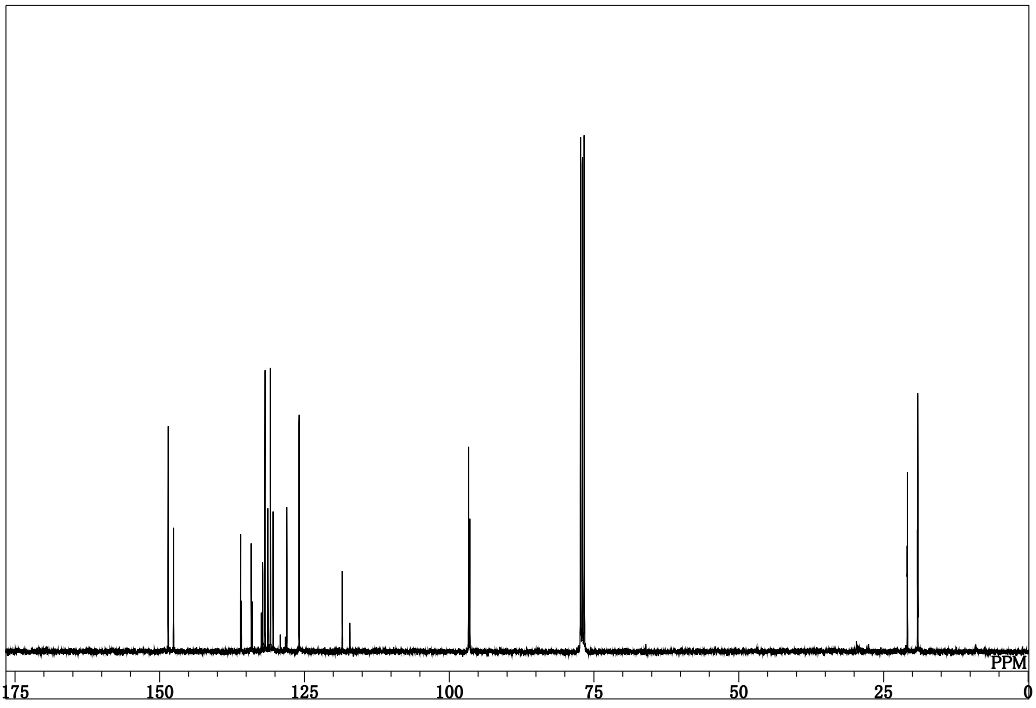


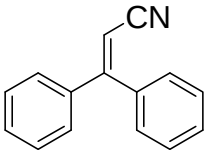




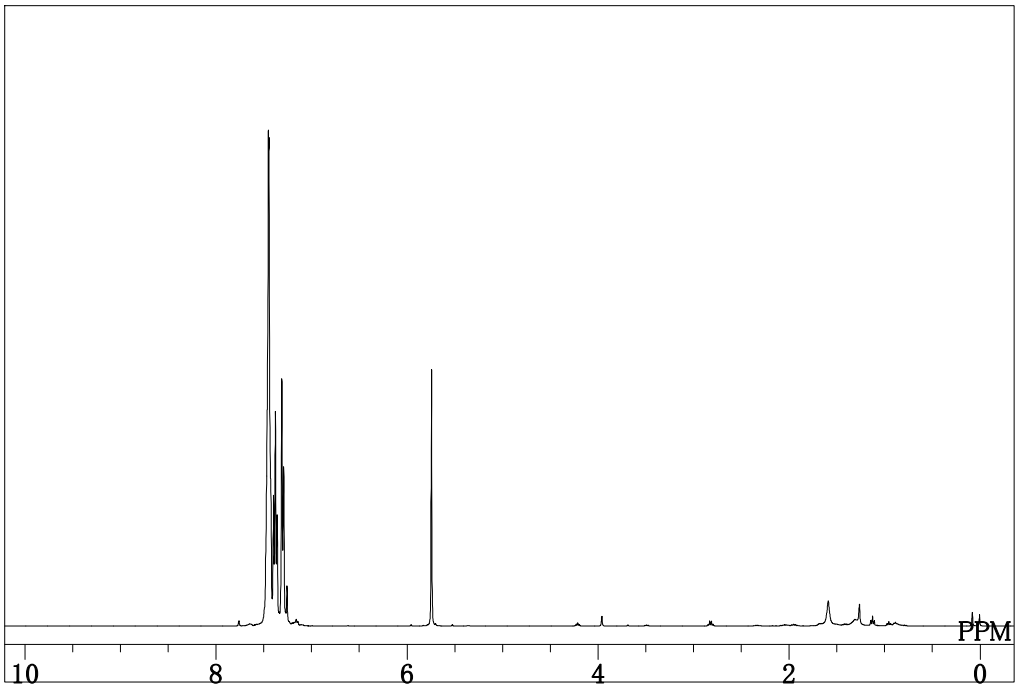
3e

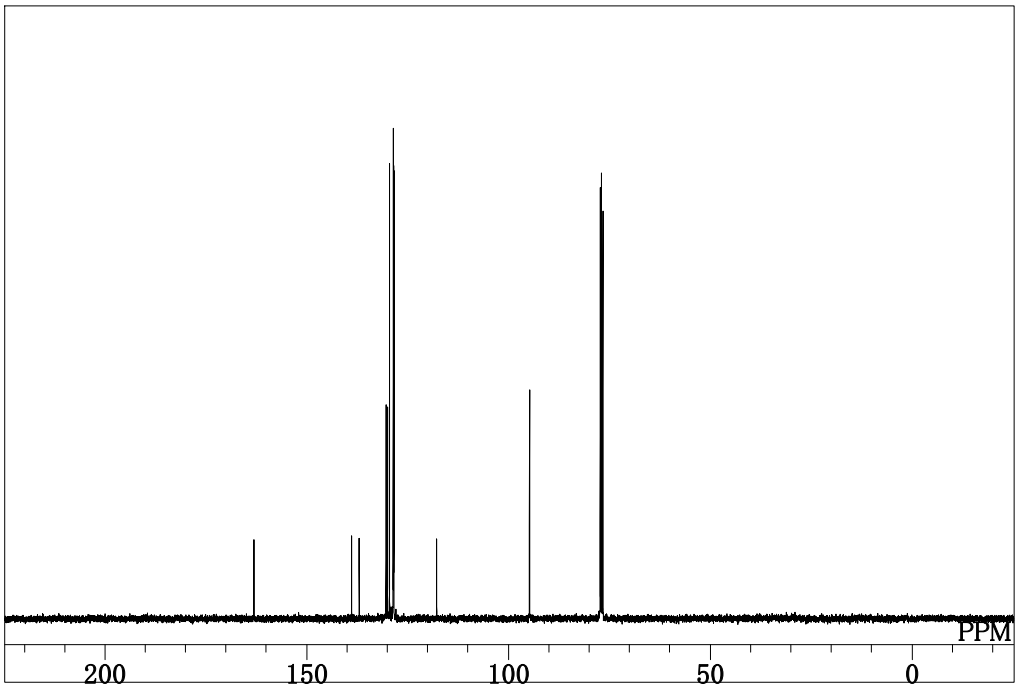


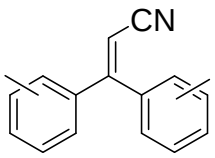




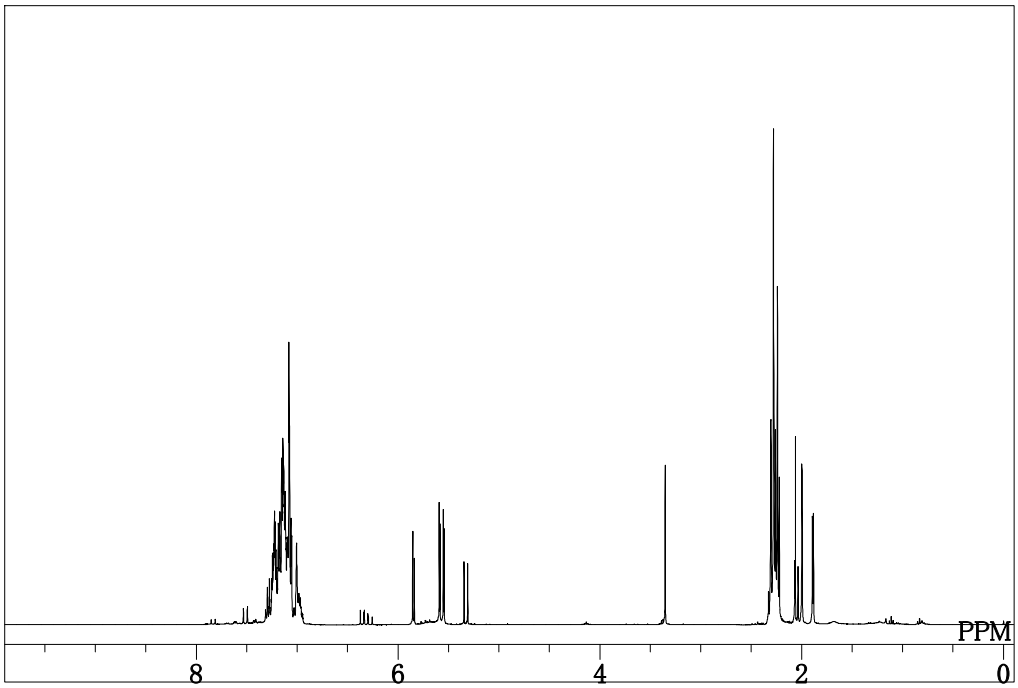
4a

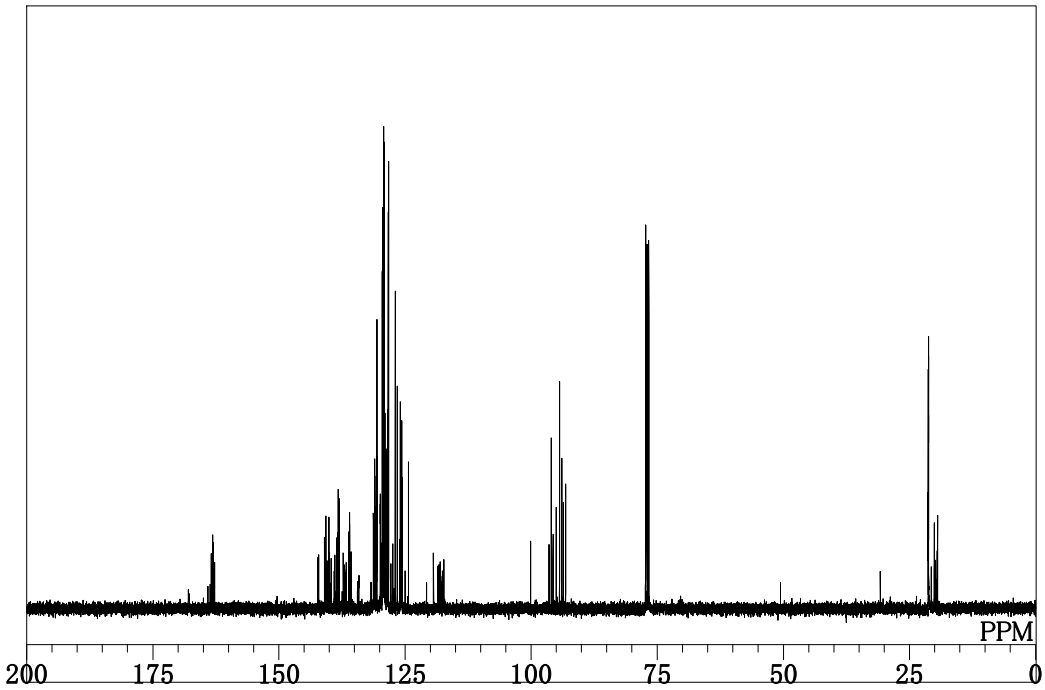


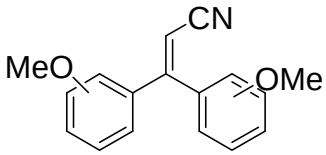




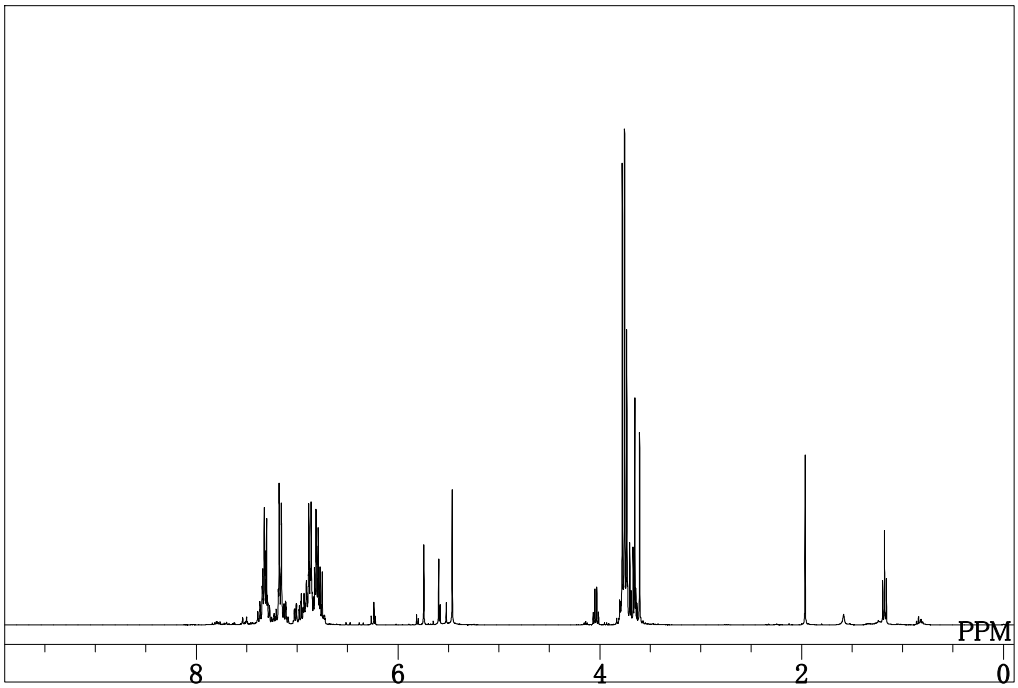
4b

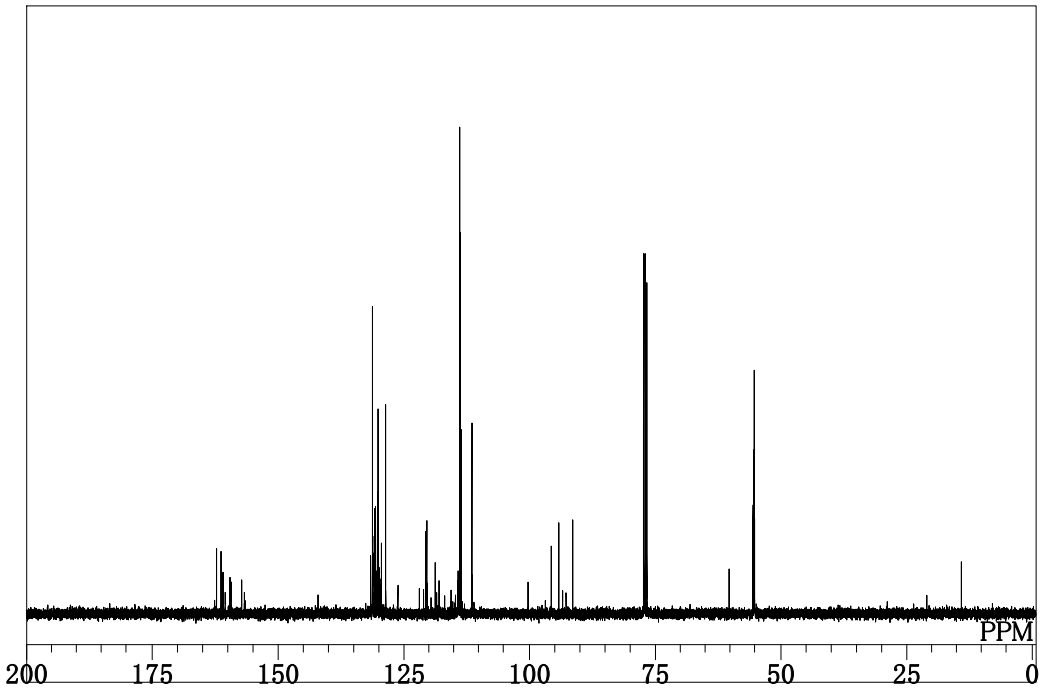


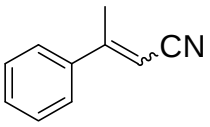




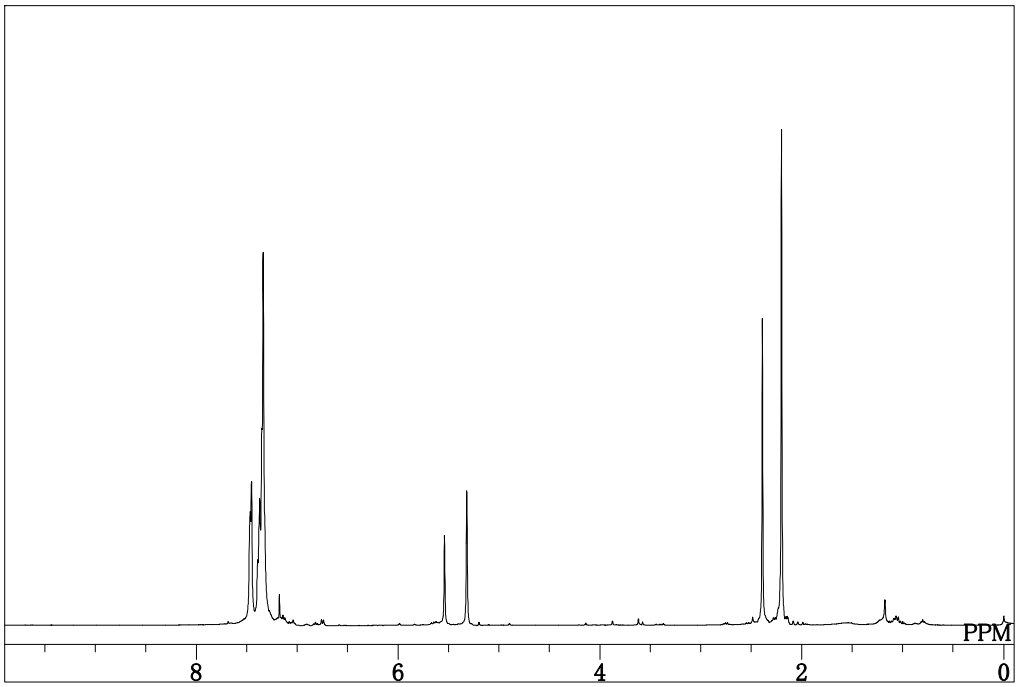
4c

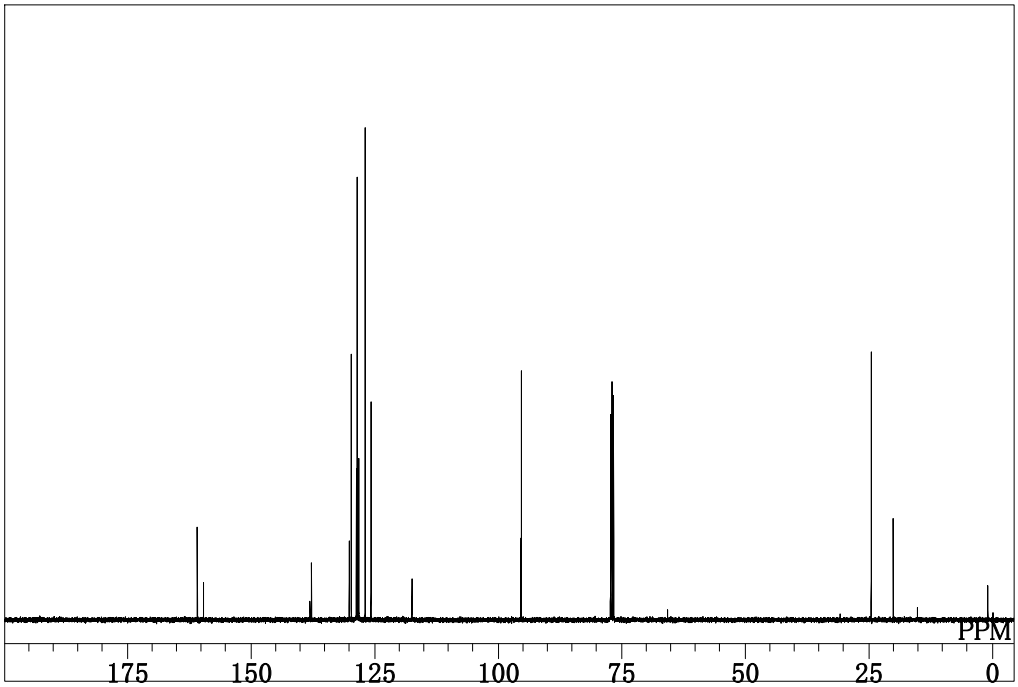


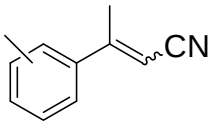




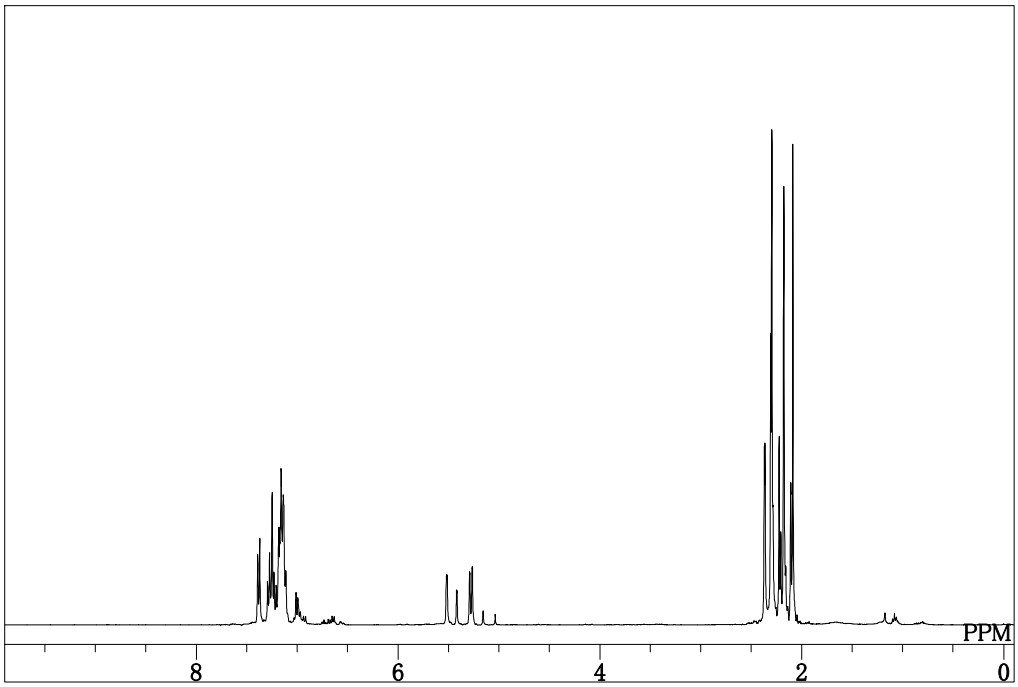
5a

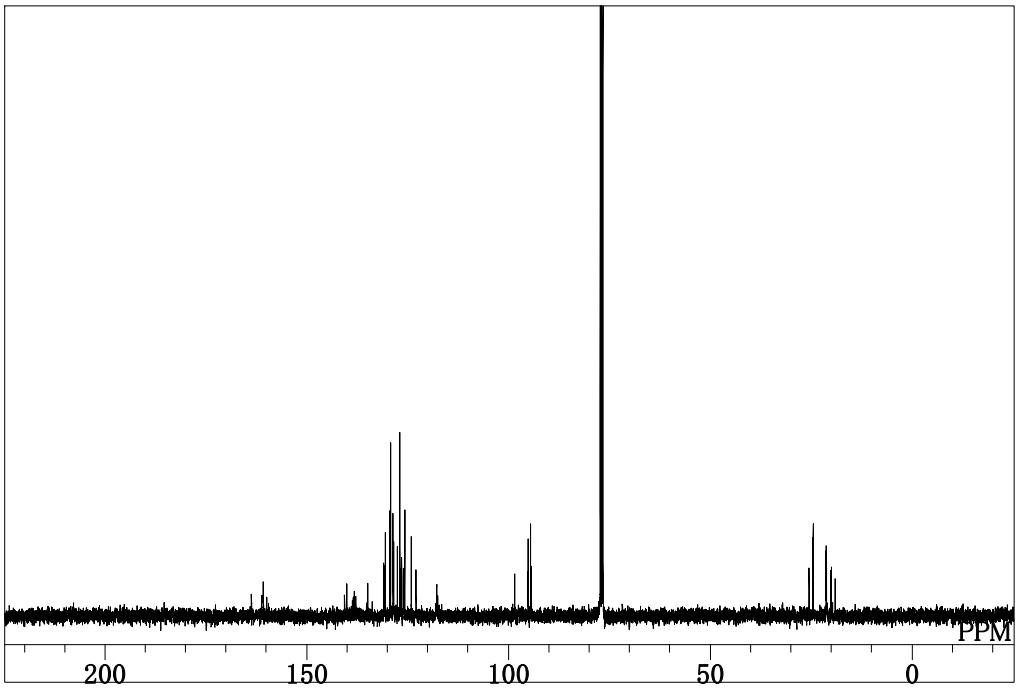


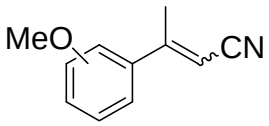




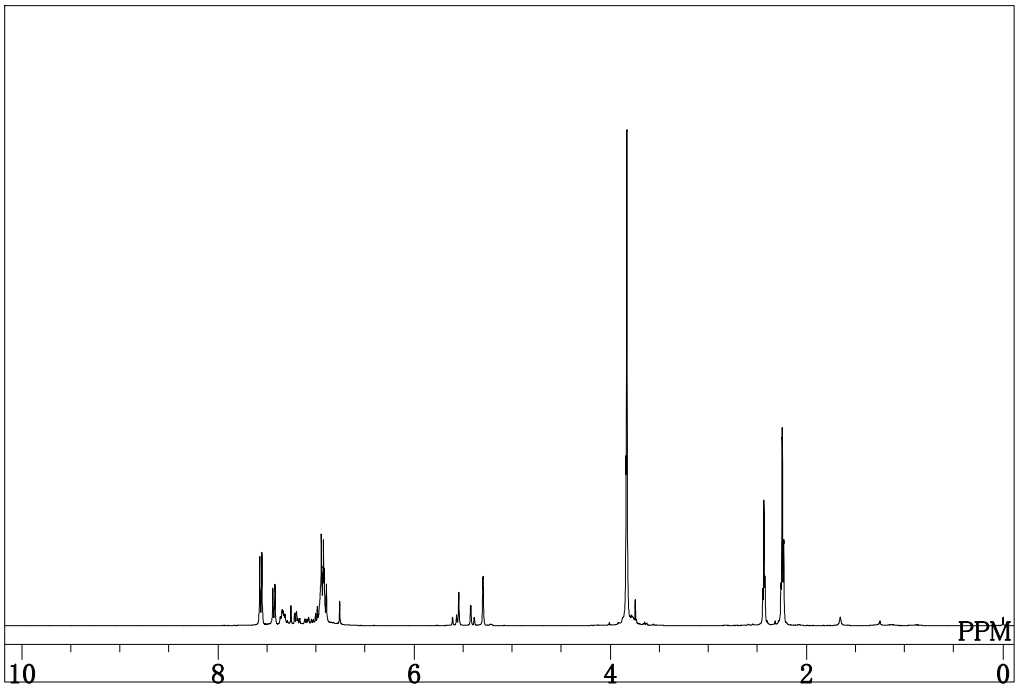
5b

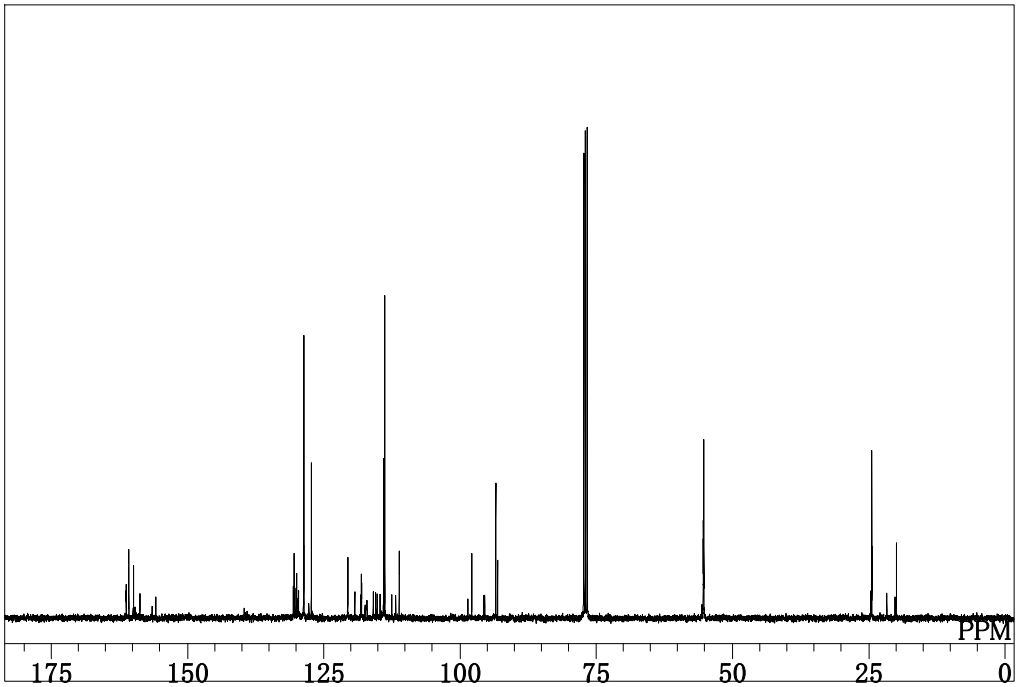


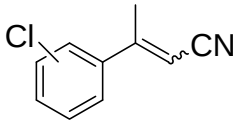




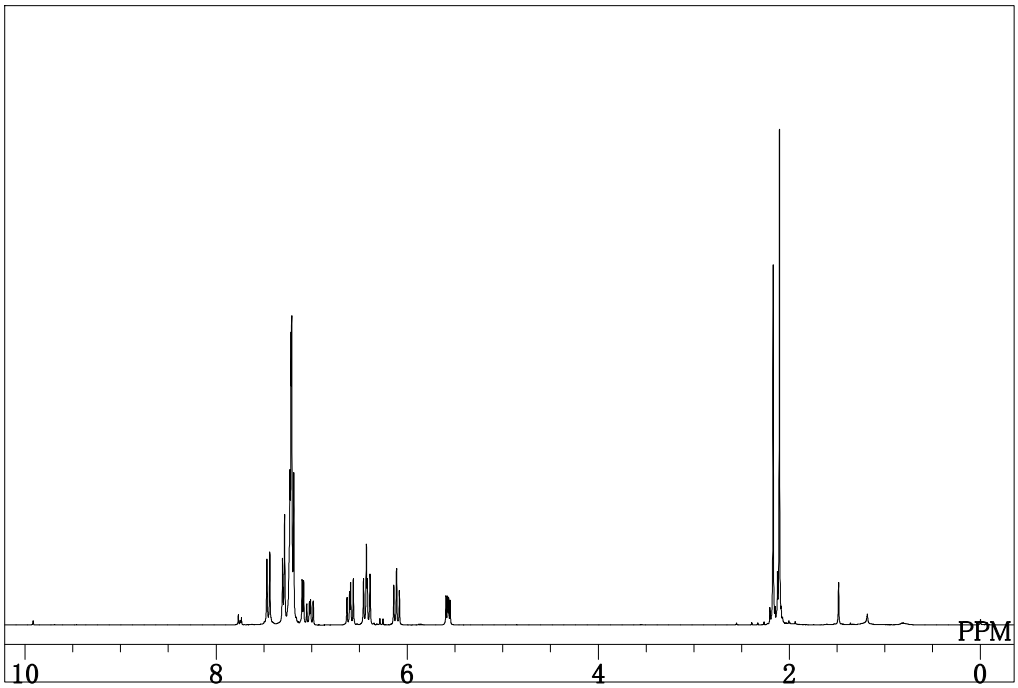
5c

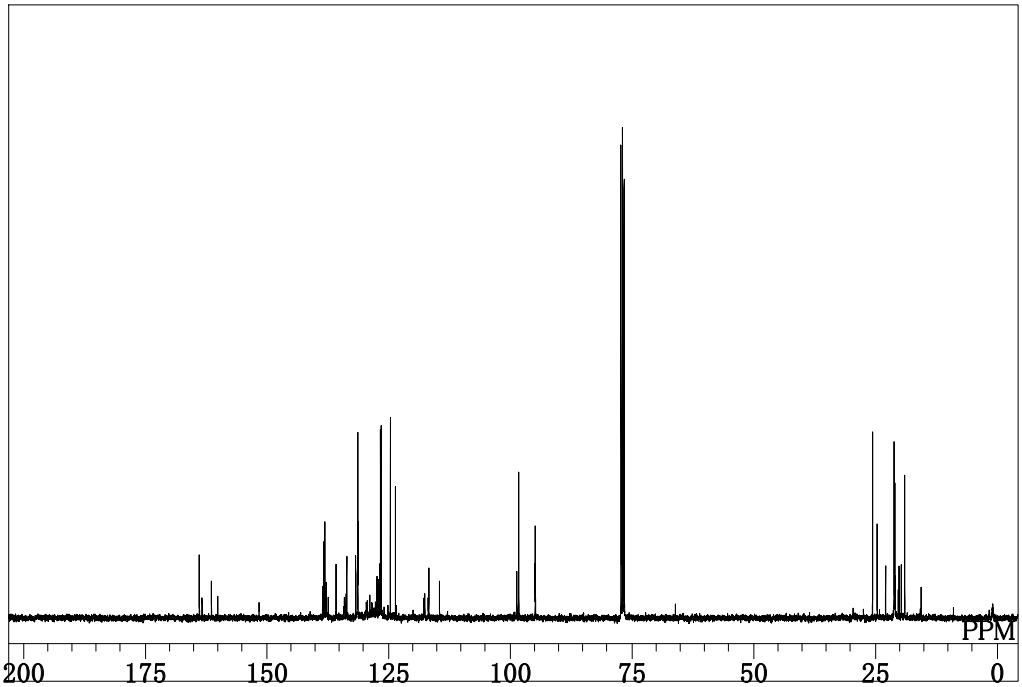


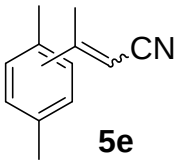




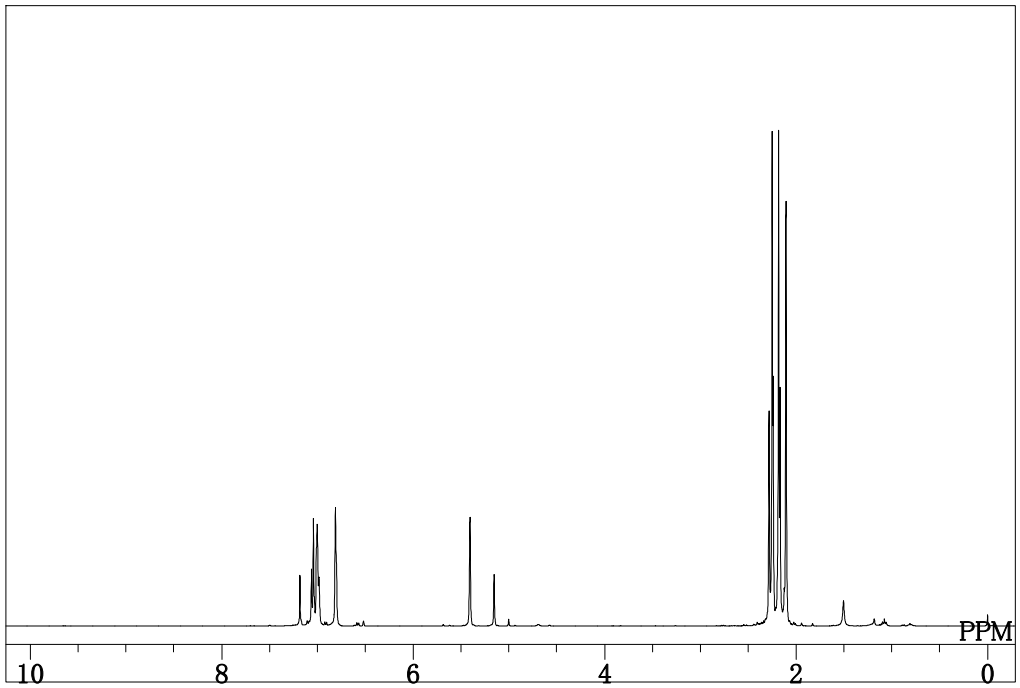
5d

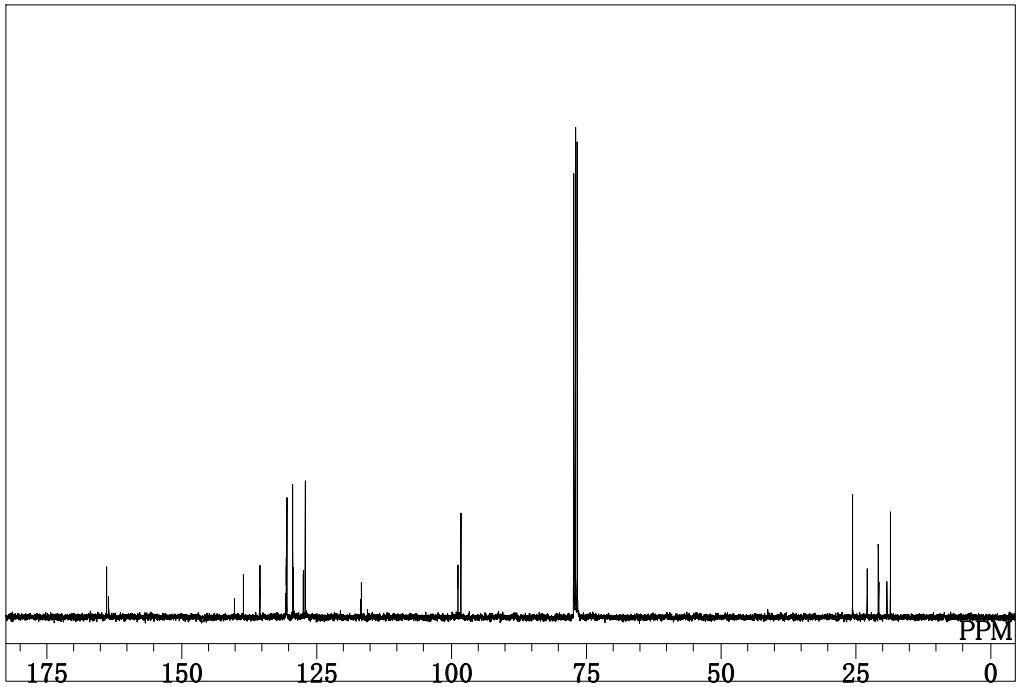


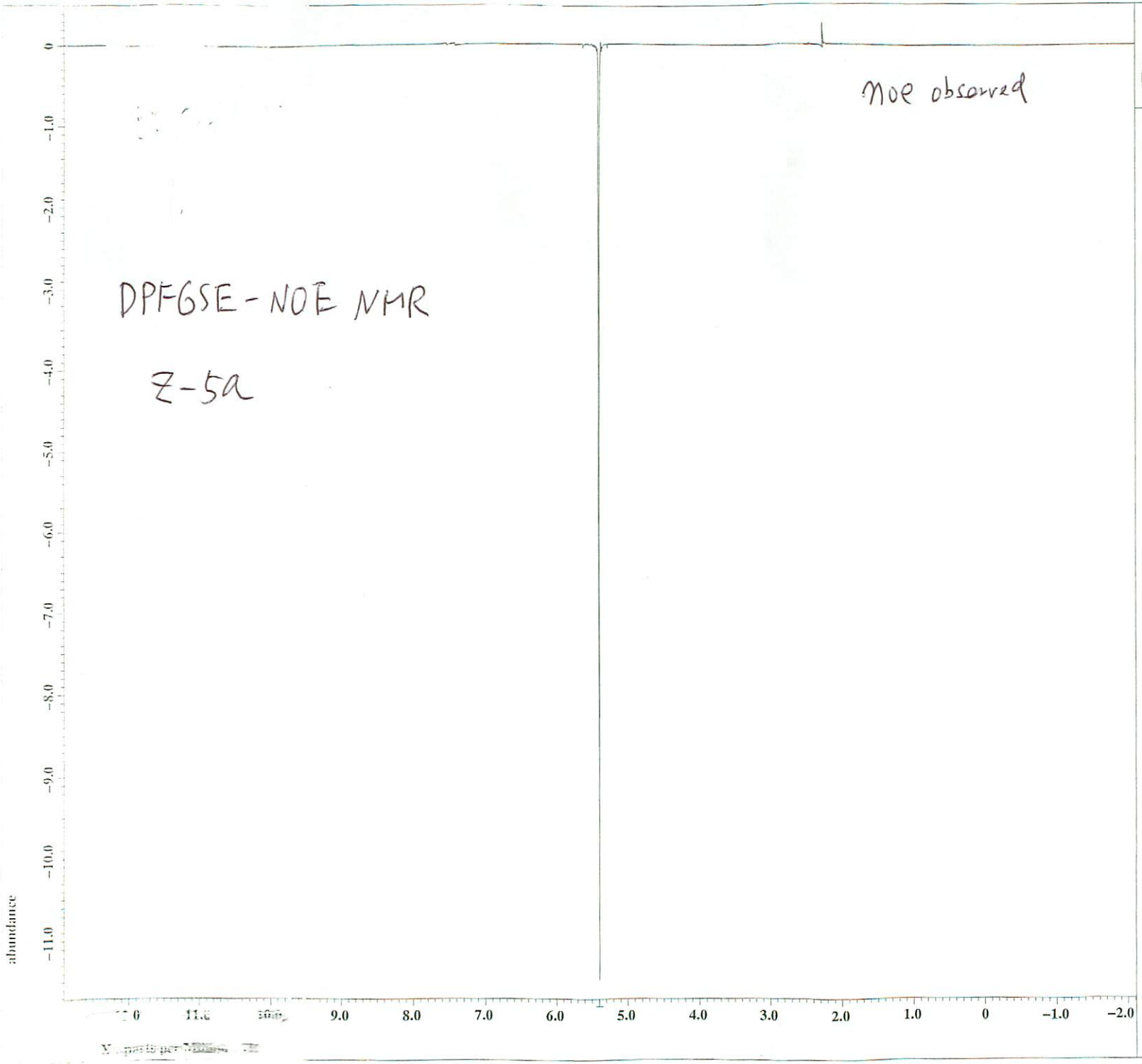




5e



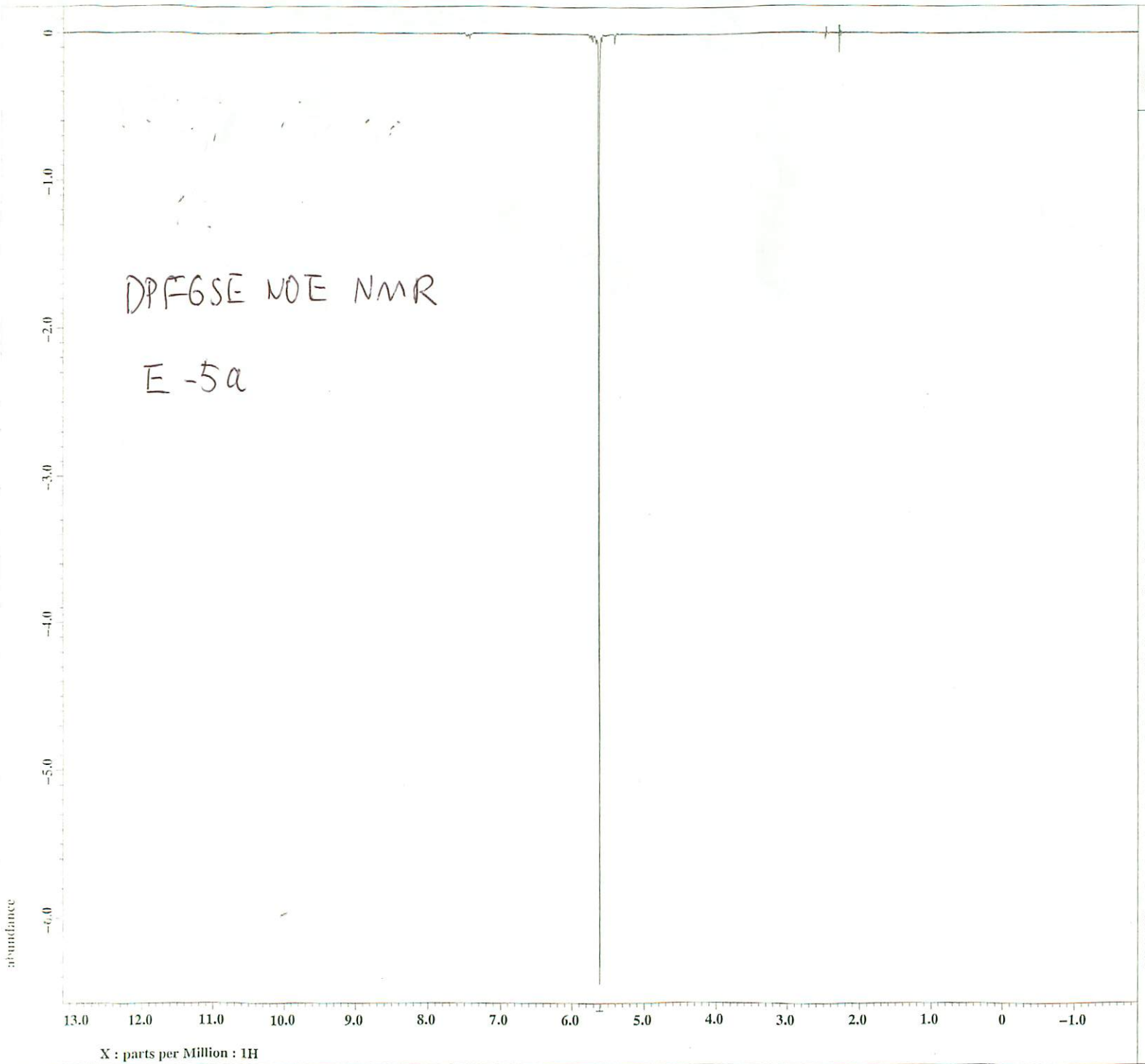




JEOL

Filename	= benzene-cro noe 5-4.j
Author	= delta
Experiment	= noe_1d_dpfgse.ex
Sample_id	= 1
Solvent	= CHLOROFORM-D
Creation_time	= 16-MAR-2010 16:24:02
Revision_time	= 16-MAR-2010 17:30:49
Current_time	= 16-MAR-2010 17:30:49
Content	= benzene-cro noe 5.392
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 400
Spectrometer	= DELTA2_NMR
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 2.18365952[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 5.3929[ppm]
X_points	= 16384
X_prescans	= 2
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_acq_time	= 2.18365952[s]
X_atn	= 6.2[dB]
X_pulse	= 11.2[us]
Irr_mode	= Off
Obs_sel_180	= 20[ms]
Obs_sel_atn	= 47.5[dB]
Obs_sel_offset	= 5.3929[ppm]
Obs_sel_shape	= GAUSS
Obs_sel_slp	= 5.3929[ppm]
Tri_mode	= Off
Dante_presat	= FALSE
Grad_1	= 1[ms]
Grad_1_amp	= 20[%]
Grad_2	= 1[ms]
Grad_2_amp	= 30[%]
Grad_3	= 1[ms]
Grad_3_amp	= 10[%]
Grad_recover	= 0.1[ms]
Grad_shape	= SINE
Initial_wait	= 1[s]
Mix_time	= 0.5[s]
Recvr_gain	= 50
Relaxation_delay	= 7[s]
Repetition_time	= 9.18365952[s]
Temp_get	= 45.2[dC]

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010



JEOL

Filename	= benzene-cro noe 5-3.j
Author	= delta
Experiment	= noe_1d_dpfgse.ex
Sample_id	= 1
Solvent	= CHLOROFORM-D
Creation_time	= 16-MAR-2010 16:21:04
Revision_time	= 16-MAR-2010 17:27:34
Current_time	= 16-MAR-2010 17:27:34
Content	= benzene-cro noe 5.615
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 400
Spectrometer	= DELTA2_NMR
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 2.18365952[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 5.6151[ppm]
X_points	= 16384
X_prescans	= 2
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 32
Total_scans	= 32
X_acq_time	= 2.18365952[s]
X_atn	= 6.2[dB]
X_pulse	= 11.2[us]
Irr_mode	= Off
Obs_sel_180	= 20[ms]
Obs_sel_atn	= 47.5[dB]
Obs_sel_offset	= 5.6151[ppm]
Obs_sel_shape	= GAUSS
Obs_sel_slp	= 5.6151[ppm]
Tri_mode	= Off
Dante_presat	= FALSE
Grad_1	= 1[ms]
Grad_1_amp	= 20[%]
Grad_2	= 1[ms]
Grad_2_amp	= 30[%]
Grad_3	= 1[ms]
Grad_3_amp	= 10[%]
Grad_recover	= 0.1[ms]
Grad_shape	= SINE
Initial_wait	= 1[s]
Mix_time	= 0.5[s]
Recvr_gain	= 50
Relaxation_delay	= 7[s]
Repetition_time	= 9.18365952[s]
Temp_get	= 45.3[dC]

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

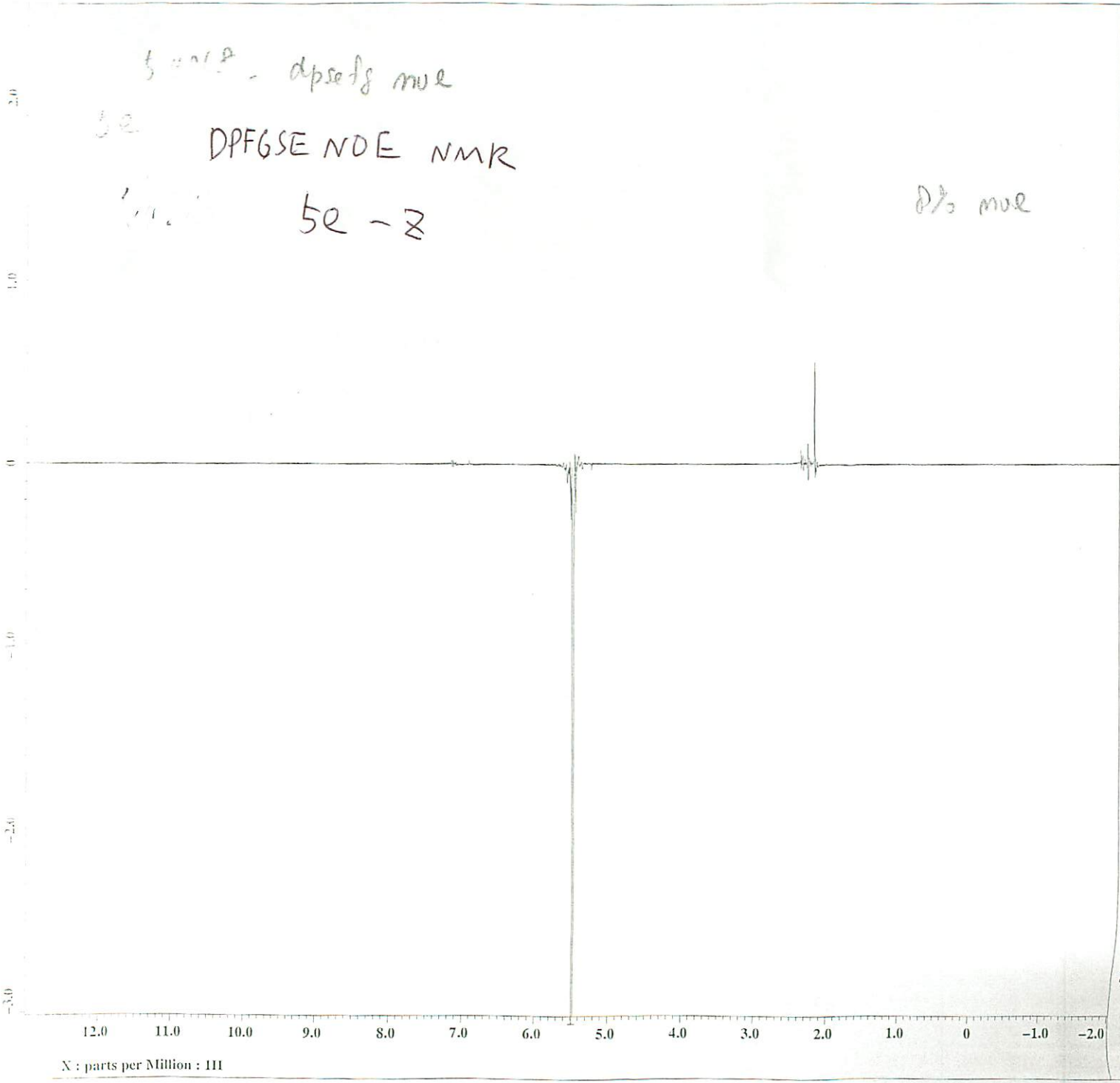
5 mg - dpfgse noe

5e

DPFGSE NOE NMR

5e - z

D2o noe



JEOL

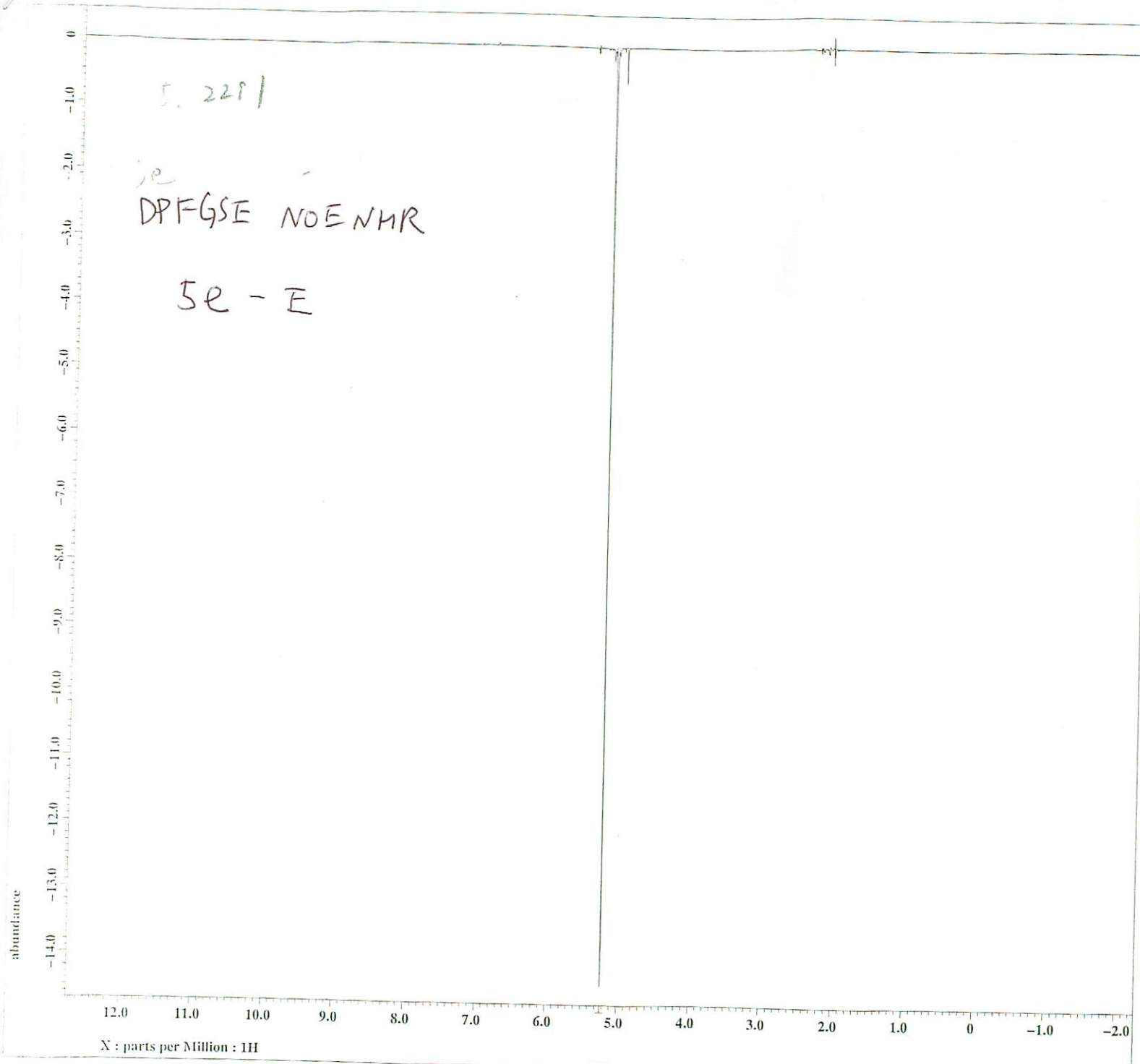
```
Filename          = P-XY-CRO NOE 5-3.jdf
Author            = delta
Experiment        = noe_1d_dpfgse.ex
Sample_id         = 1
Solvent           = CHLOROFORM-D
Creation_time     =  4-MAR-2010 12:05:34
Revision_time     =  4-MAR-2010 13:14:15
Current_time      =  4-MAR-2010 13:14:15

Content           = P-XY-CRO NOE 5.4868
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 400
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 2.18365952[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5.4868[ppm]
X_points          = 16384
X_prescans        = 2
X_resolution      = 0.45794685[Hz]
X_sweep           = 7.5030012[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_acq_time        = 2.18365952[s]
X_atn             = 6.2[dB]
X_pulse           = 11.2[us]
Irr_mode          = Off
Obs_sel_180       = 20[ms]
Obs_sel_atn       = 47.5[dB]
Obs_sel_offset    = 5.4868[ppm]
Obs_sel_shape     = GAUSS
Obs_sel_slp       = 5.4868[ppm]
Tri_mode          = Off
Dante_presat      = FALSE
Grad_1            = 1[ms]
Grad_1_amp        = 20[%]
Grad_2            = 1[ms]
Grad_2_amp        = 30[%]
Grad_3            = 1[ms]
Grad_3_amp        = 10[%]
Grad_recover      = 0.1[ms]
Grad_shape        = SINE
Initial_wait      = 1[s]
Mix_time          = 0.5[s]
Recvr_gain        = 50
Relaxation_delay  = 7[s]
Repetition_time   = 9.18365952[s]
Temp_get          = 39.4[dC]
```

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010



JEOL

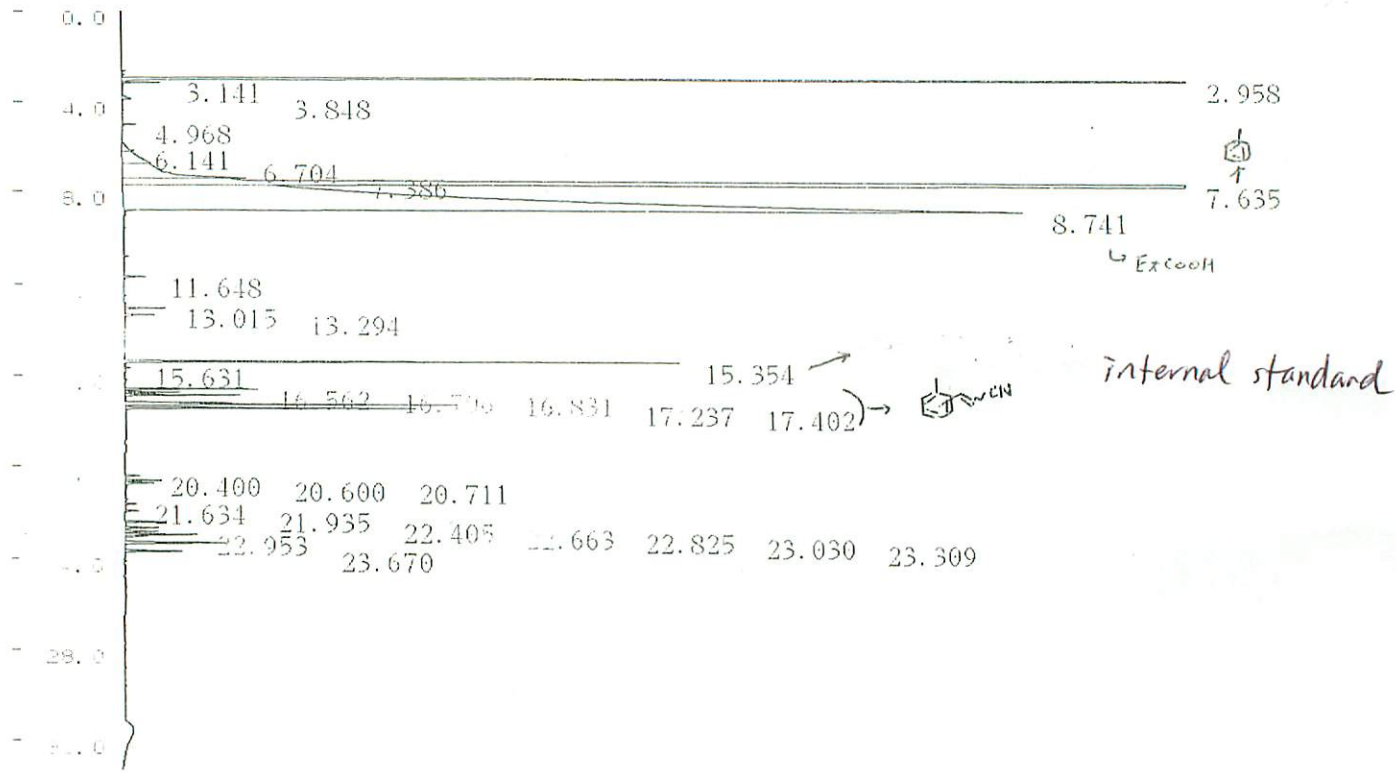
Filename	= P-XY-CRO NOE 5.{-3.jd
Author	= delta
Experiment	= noe_1d_dpfgse.ex
Sample_id	= 1
Solvent	= CHLOROFORM-D
Creation_time	= 4-MAR-2010 12:12:47
Revision_time	= 4-MAR-2010 13:20:30
Current_time	= 4-MAR-2010 13:20:30
Content	= P-XY-CRO NOE 5.2291
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECA 400
Spectrometer	= DELTA2_NMR
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 2.18365952[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 5.2291[ppm]
X_points	= 16384
X_prescans	= 2
X_resolution	= 0.45794685[Hz]
X_sweep	= 7.5030012[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_acq_time	= 2.18365952[s]
X_atn	= 6.2[dB]
X_pulse	= 11.2[us]
Irr_mode	= Off
Obs_sel_180	= 20[ms]
Obs_sel_atn	= 47.5[dB]
Obs_sel_offset	= 5.2291[ppm]
Obs_sel_shape	= GAUSS
Obs_sel_slp	= 5.2291[ppm]
Tri_mode	= Off
Dante_presat	= FALSE
Grad_1	= 1[ms]
Grad_1_amp	= 20[%]
Grad_2	= 1[ms]
Grad_2_amp	= 30[%]
Grad_3	= 1[ms]
Grad_3_amp	= 10[%]
Grad_recover	= 0.1[ms]
Grad_shape	= SINE
Initial_wait	= 1[s]
Mix_time	= 0.5[s]
Recvr_gain	= 50
Relaxation_delay	= 7[s]
Repetition_time	= 9.18365952[s]
Temp_get	= 38.8[dC]

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

Table 2

entry 2

CHROMATOPAC C-R7A CH=1 REPORT No.=11 ﾌｧｲﾙ=2:7100KA.C00 08/09/09 18:01:40



** 定量計算結果 **

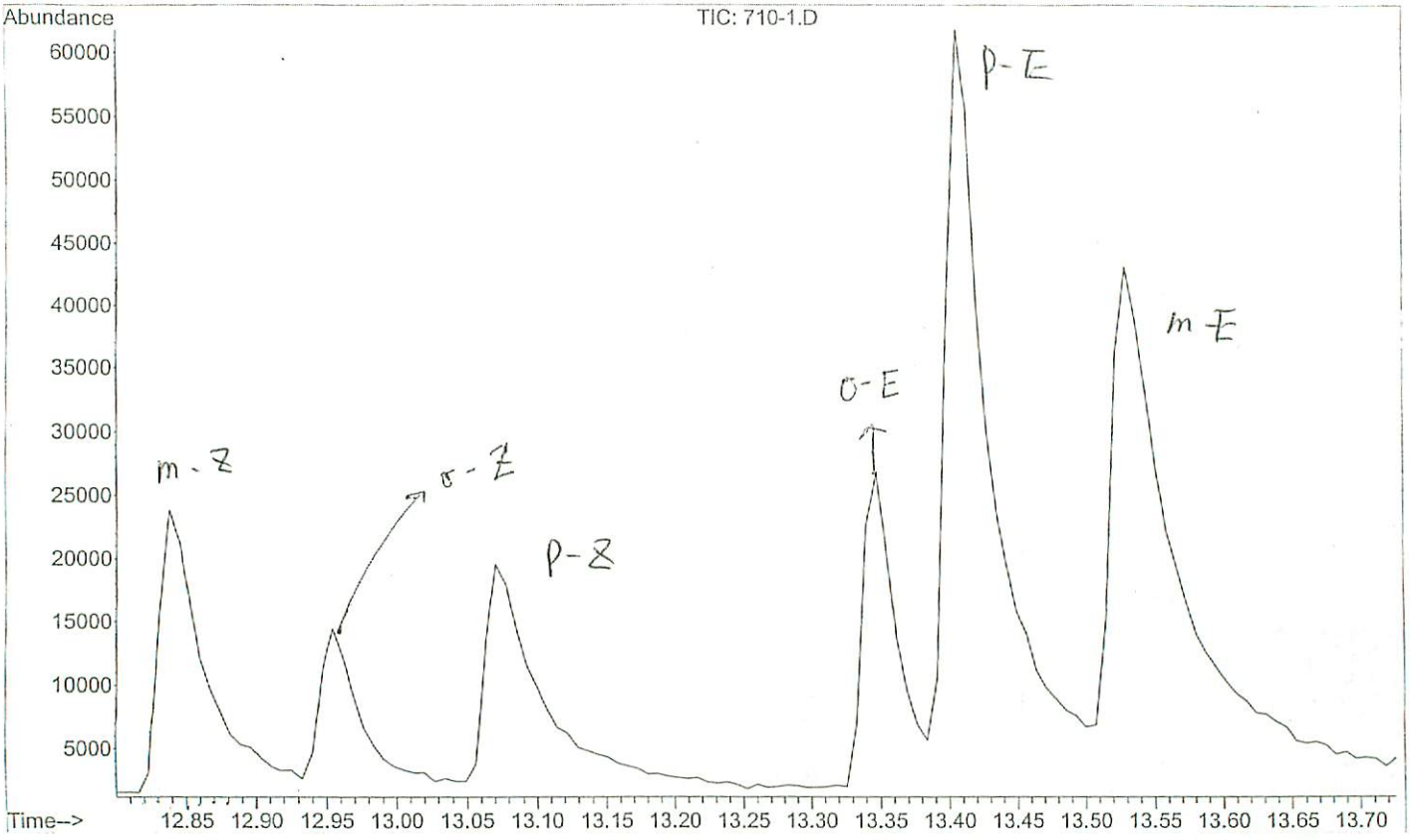
CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	3	2.958	1970702	930870	V		30.0559	
	4	3.141	3847	2048	L		0.0587	
	5	3.848	3201	518	L		0.0488	
	7	4.968	3528	823	V		0.0538	
	8	6.141	8313	729			0.1268	
	9	6.704	35818	1685	V		0.5463	
	10	7.386	124366	7246	V		1.8968	
	11	7.635	2478334	471984	V		37.798	
	12	8.741	1586764	54116	SV		24.2003	
	16	11.648	3349	1267			0.0511	
	20	13.015	6054	2417	V		0.0923	
	21	13.294	5989	1780	V		0.0913	
	23	15.354	84536	33164			1.2893	
	24	15.631	1038	333	V		0.0158	
	27	16.562	18633	7814			0.2842	
	28	16.706	7976	3229	V		0.1216	
	29	16.831	16734	6754	V		0.2552	
	30	17.237	64969	19461			0.9909	
	31	17.402	43619	17075	V		0.6653	
	35	20.4	3679	834			0.0409	
	36	20.6	557	2117	V		0.1	
	37	20.711	6067	1667	V		0.0925	
	41	21.634	2321	673			0.0308	
	43	21.935	2591	803	V		0.0395	
	44	22.405	6695	2370			0.1021	
	45	22.663	6007	1920			0.0916	
	46	22.825	5746	1922	V		0.0876	
	47	22.953	13009	4249	V		0.1984	
	48	23.03	3592	1309	V		0.0548	
	49	23.309	23696	5847			0.3611	
	50	-	10357	3301			0.158	
		TOTAL	6556782	1590319			100	

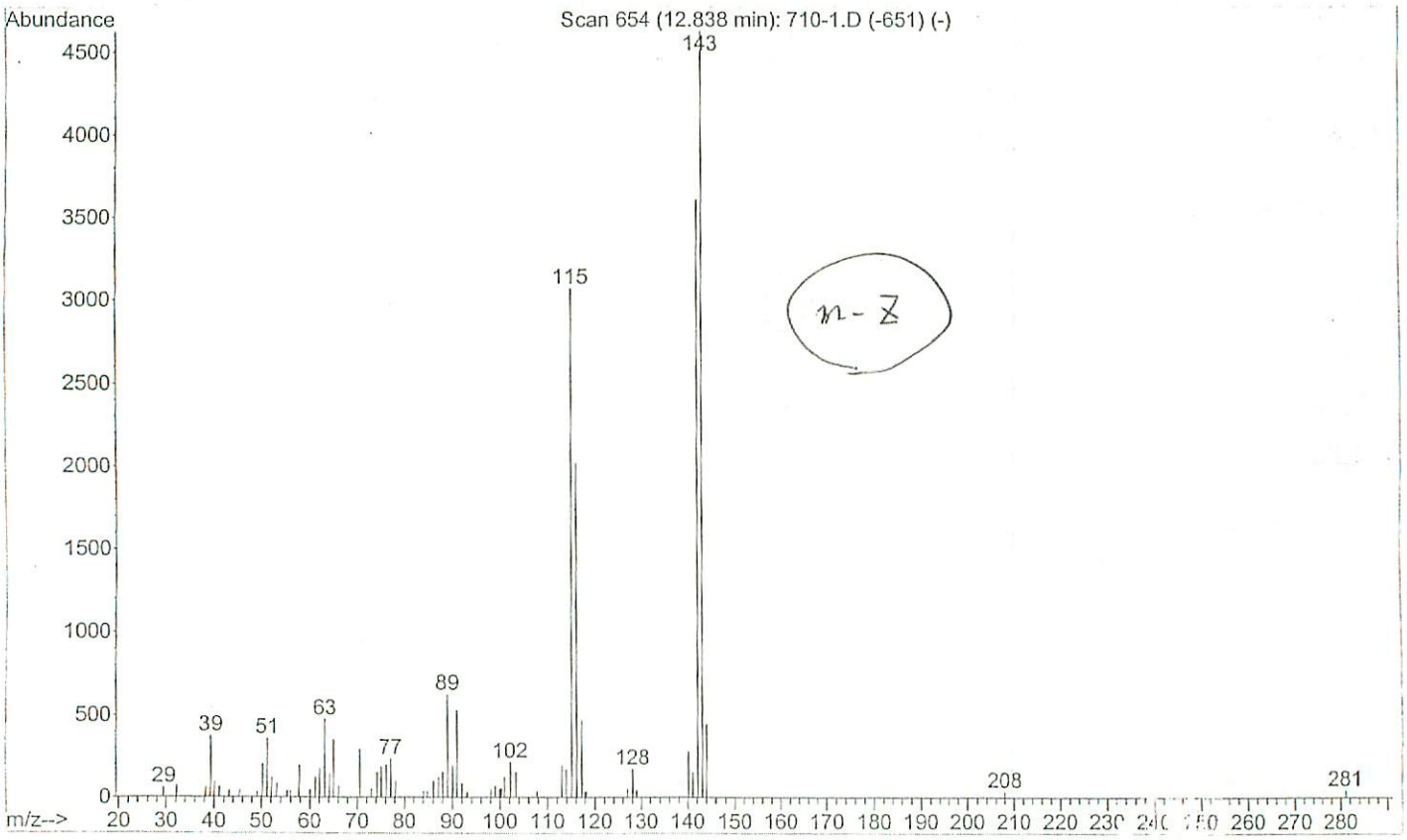
m-Z
o-Z
p-Z
o-E
p-E
m-E

64969 0.9909

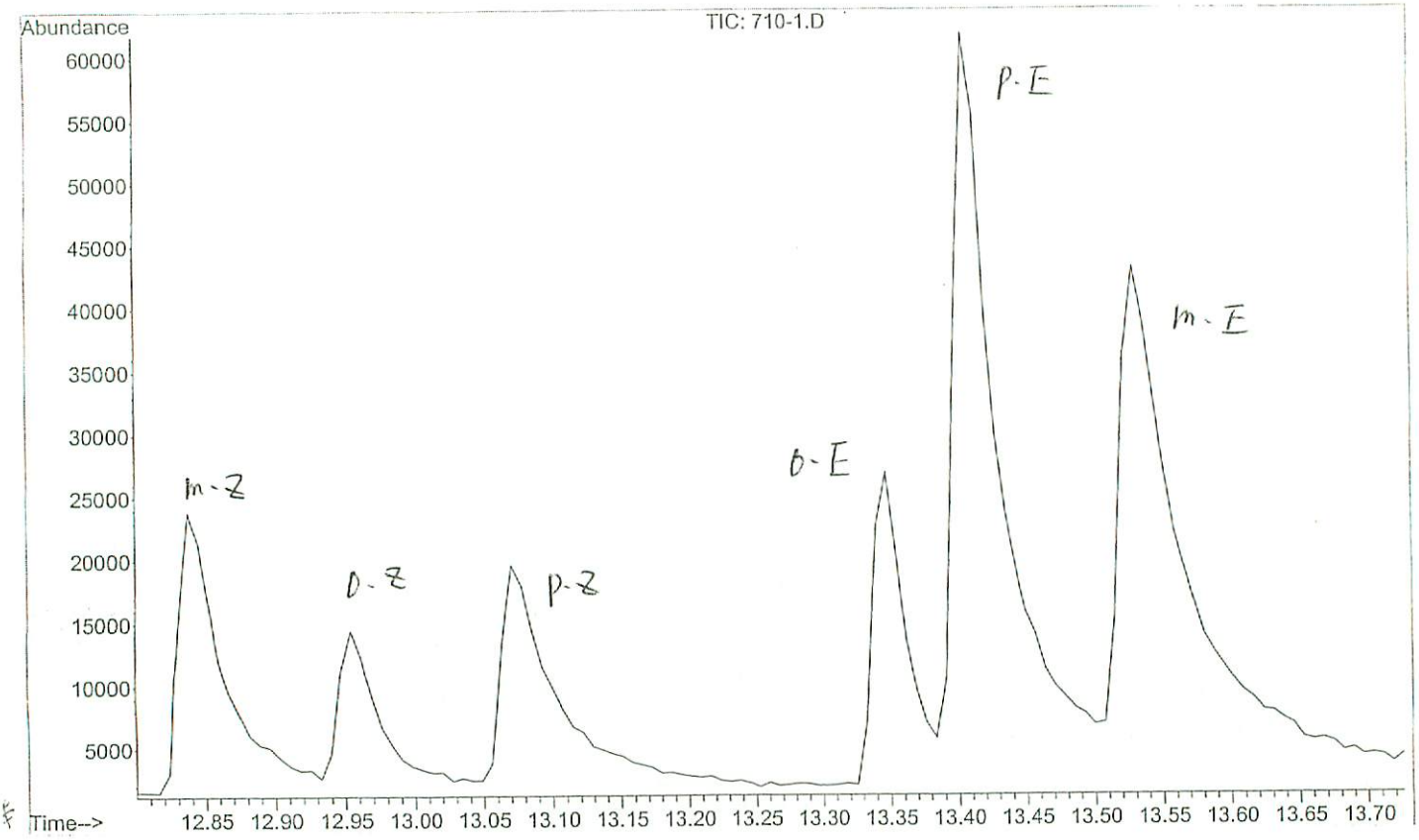
64969 x 0.6653 / 0.9909

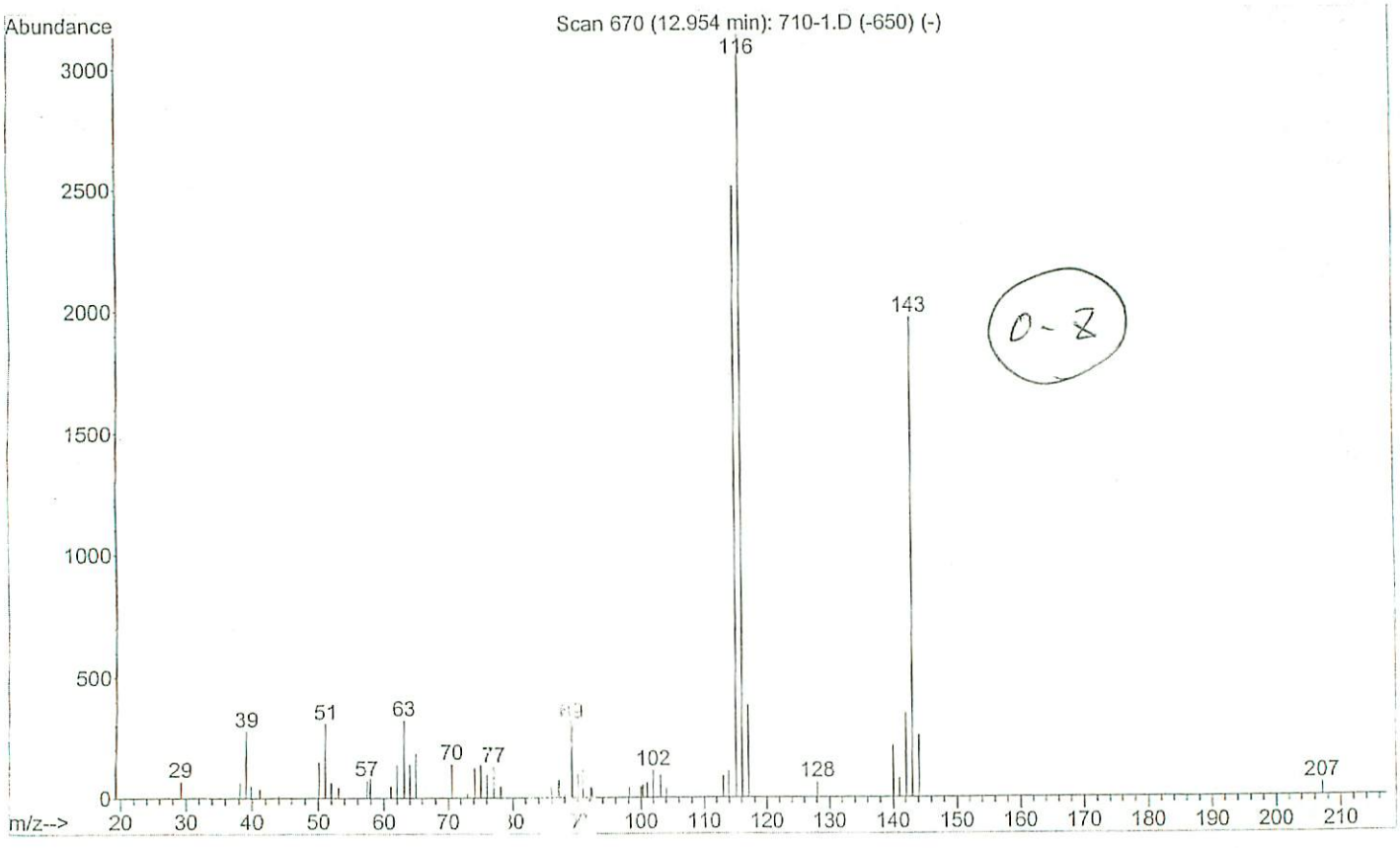
7JD

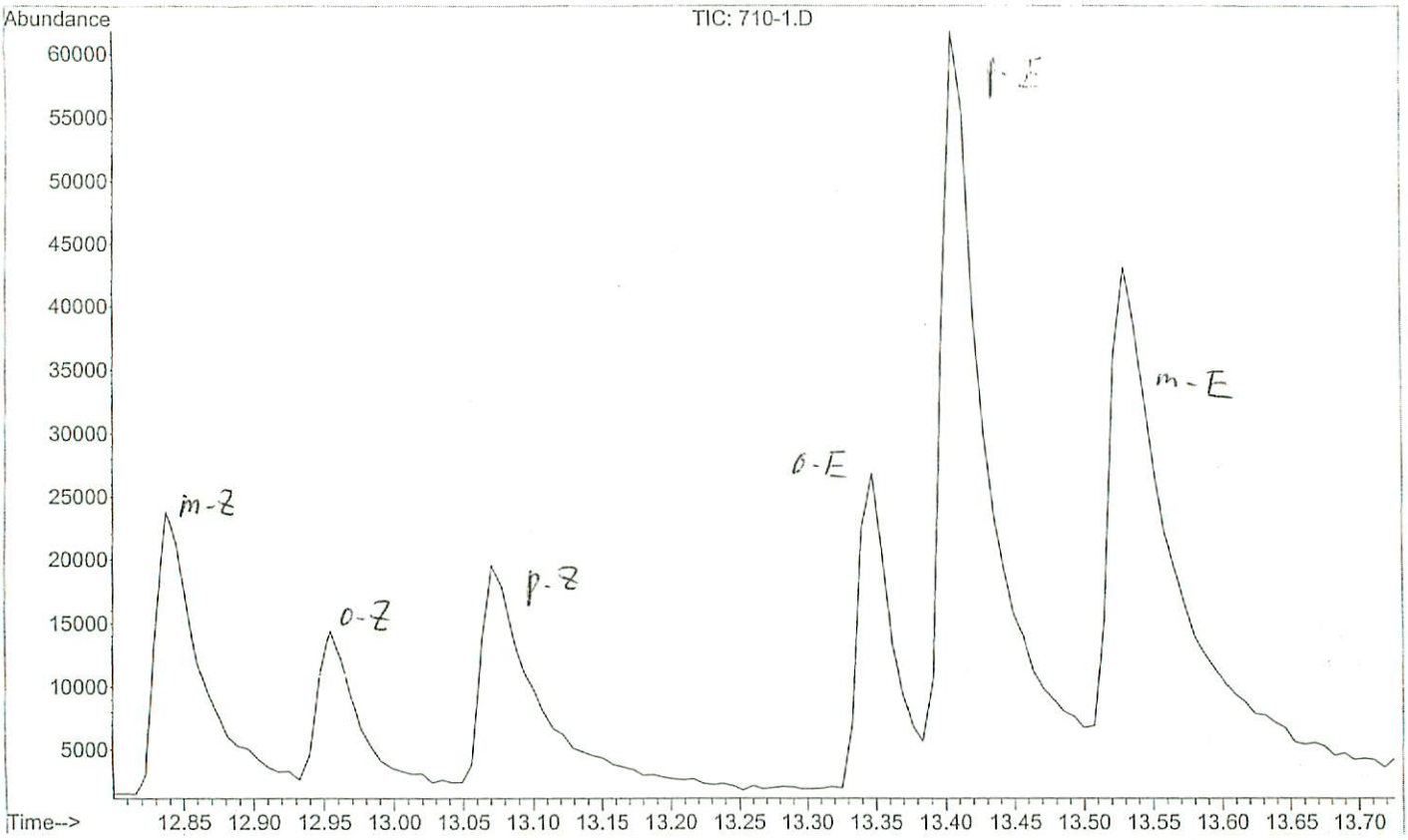

Abundance
TIC: 710-1.D
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
m-Z
o-Z
p-Z
o-E
p-E
m-E
Time-->
12.85 12.90 12.95 13.00 13.05 13.10 13.15 13.20 13.25 13.30 13.35 13.40 13.45 13.50 13.55 13.60 13.65 13.70

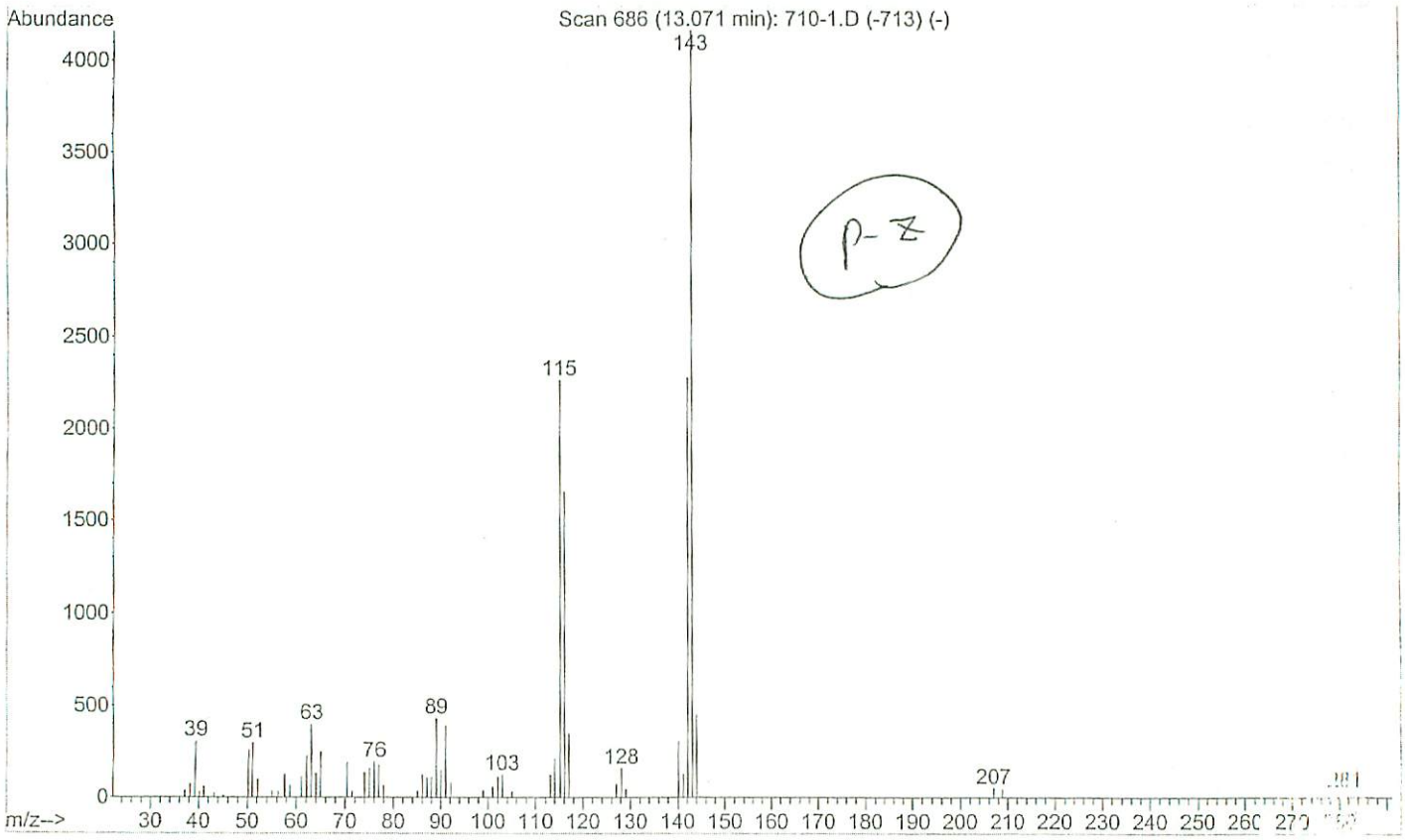

Abundance
Scan 654 (12.838 min): 710-1.D (-651) (-)
4500
4000
3500
3000
2500
2000
1500
1000
500
0
143
115
m-Z
89
63
39
51
77
102
128
29
208
281
m/z-->
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280

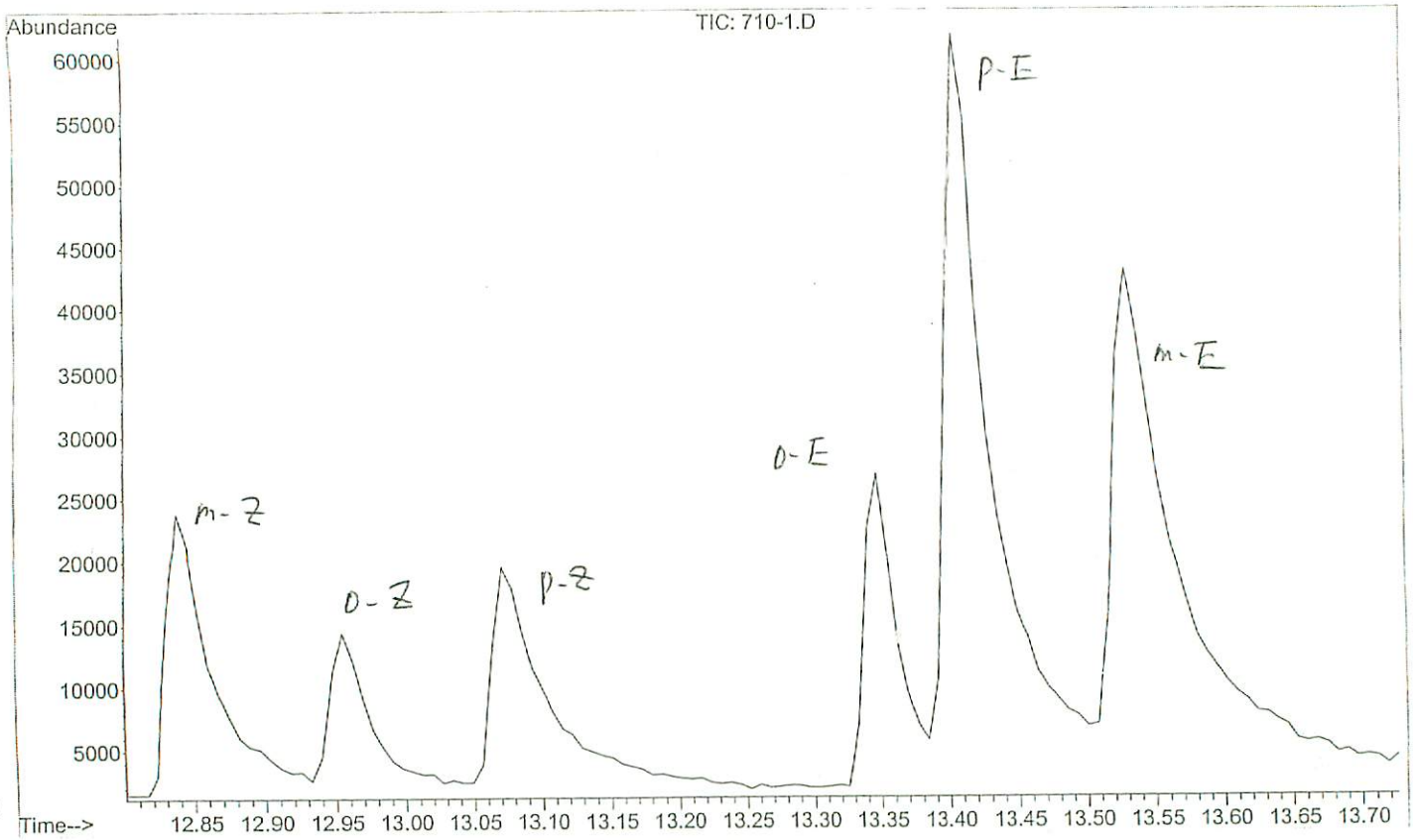
This journal is (c) The Royal Society of Chemistry 2010

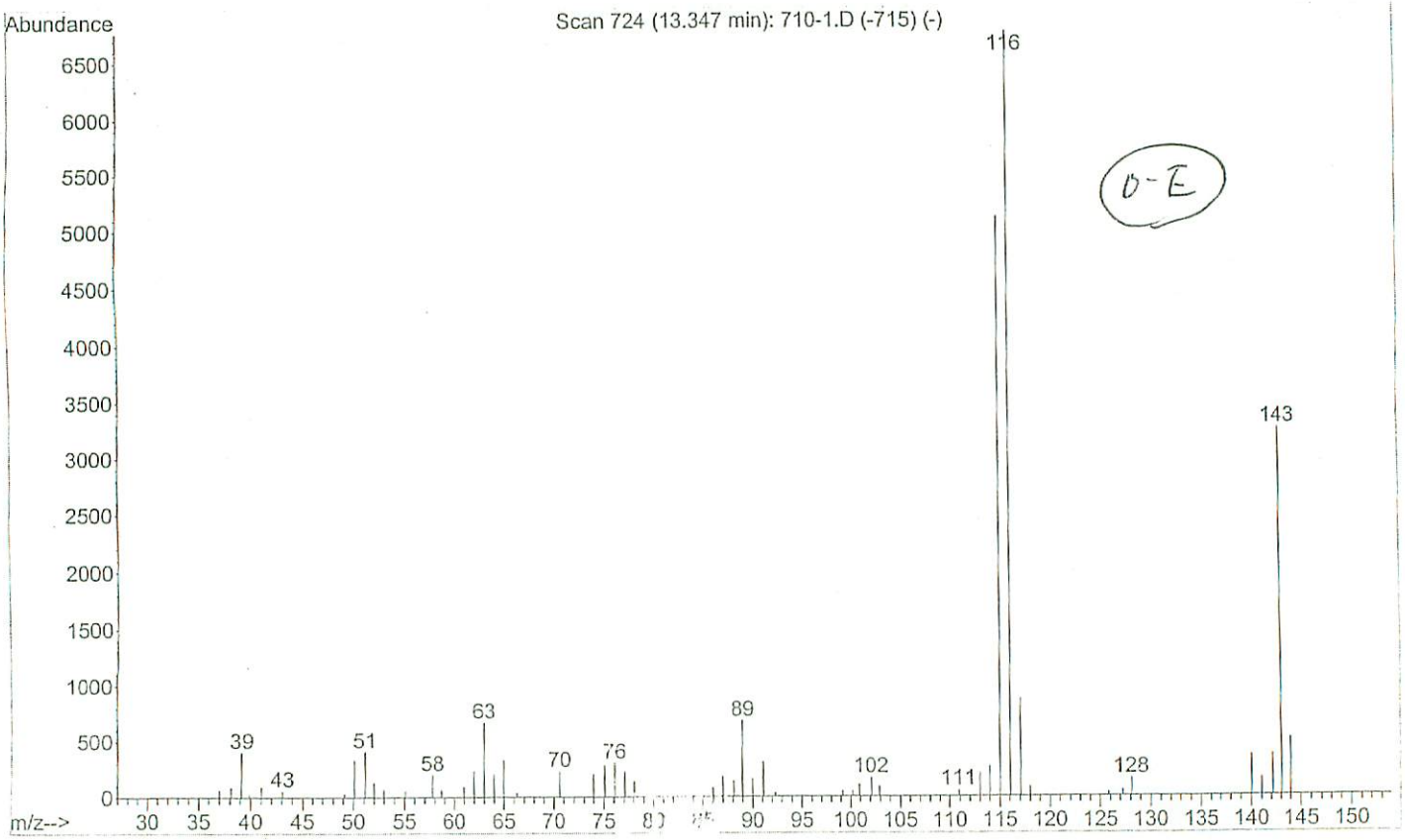


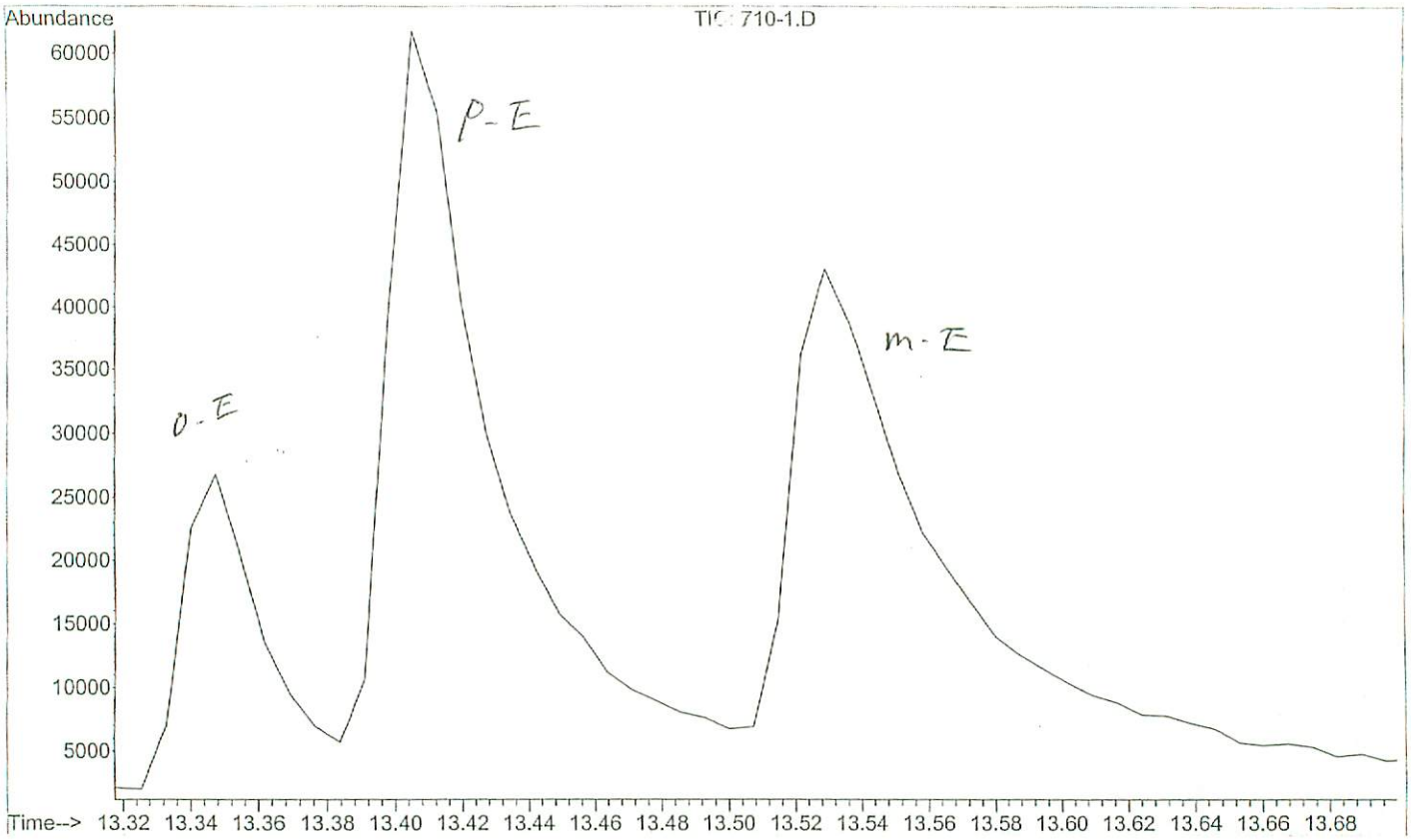


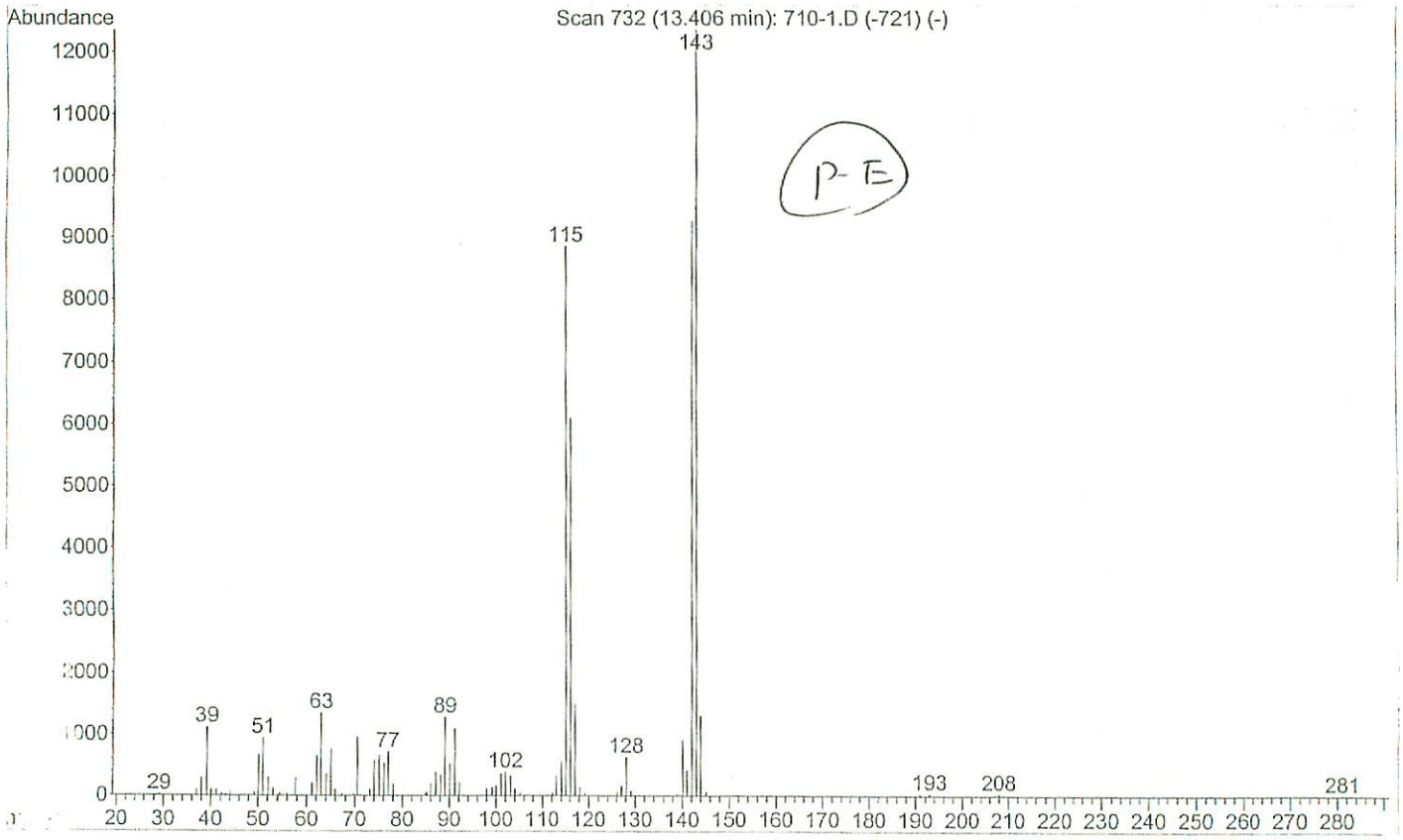

Abundance
TIC: 710-1.D
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
m-Z
o-Z
p-Z
o-E
p-E
m-E
Time-->
12.85 12.90 12.95 13.00 13.05 13.10 13.15 13.20 13.25 13.30 13.35 13.40 13.45 13.50 13.55 13.60 13.65 13.70

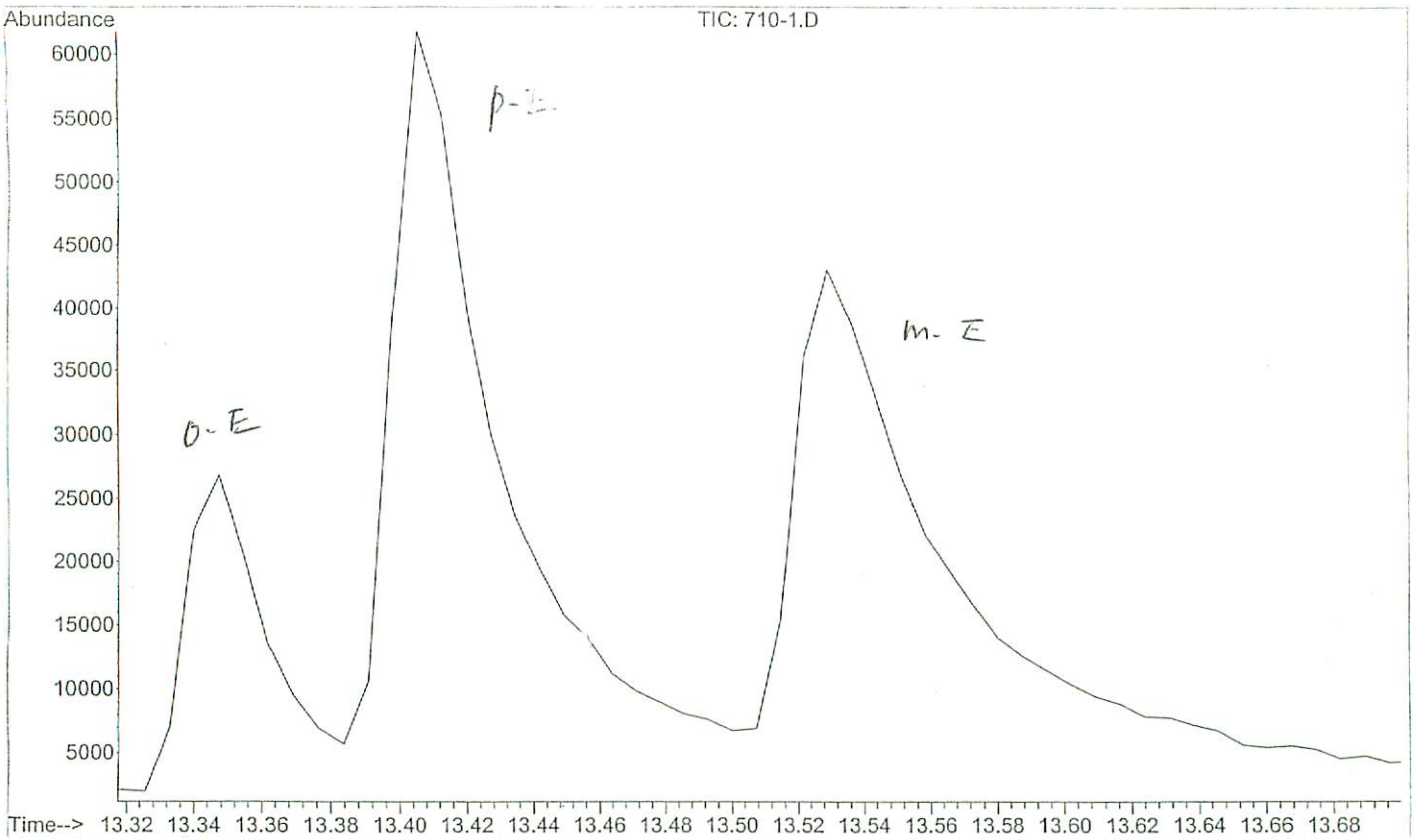

Abundance
Scan 686 (13.071 min): 710-1.D (-713) (-)
4000
3500
3000
2500
2000
1500
1000
500
0
143
115
p-Z
39
51
63
76
89
103
128
207
m/z-->
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270


TIC: 710-1.D
Abundance
Time-->
m-Z
o-Z
p-Z
o-E
p-E
m-E


Scan 724 (13.347 min): 710-1.D (-715) (-)
Abundance
m/z-->
o-E
116
143
89
63
39
51
58
70
76
43
102
111
128


Abundance
TIC: 710-1.D
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
p-E
o-E
m-E
Time--> 13.32 13.34 13.36 13.38 13.40 13.42 13.44 13.46 13.48 13.50 13.52 13.54 13.56 13.58 13.60 13.62 13.64 13.66 13.68


Abundance
Scan 732 (13.406 min): 710-1.D (-721) (-)
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
143
115
p-E
39
51
63
77
89
102
128
29
193
208
281
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280


Abundance
TIC: 710-1.D
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
p-E
m-E
o-E
Time--> 13.32 13.34 13.36 13.38 13.40 13.42 13.44 13.46 13.48 13.50 13.52 13.54 13.56 13.58 13.60 13.62 13.64 13.66 13.68

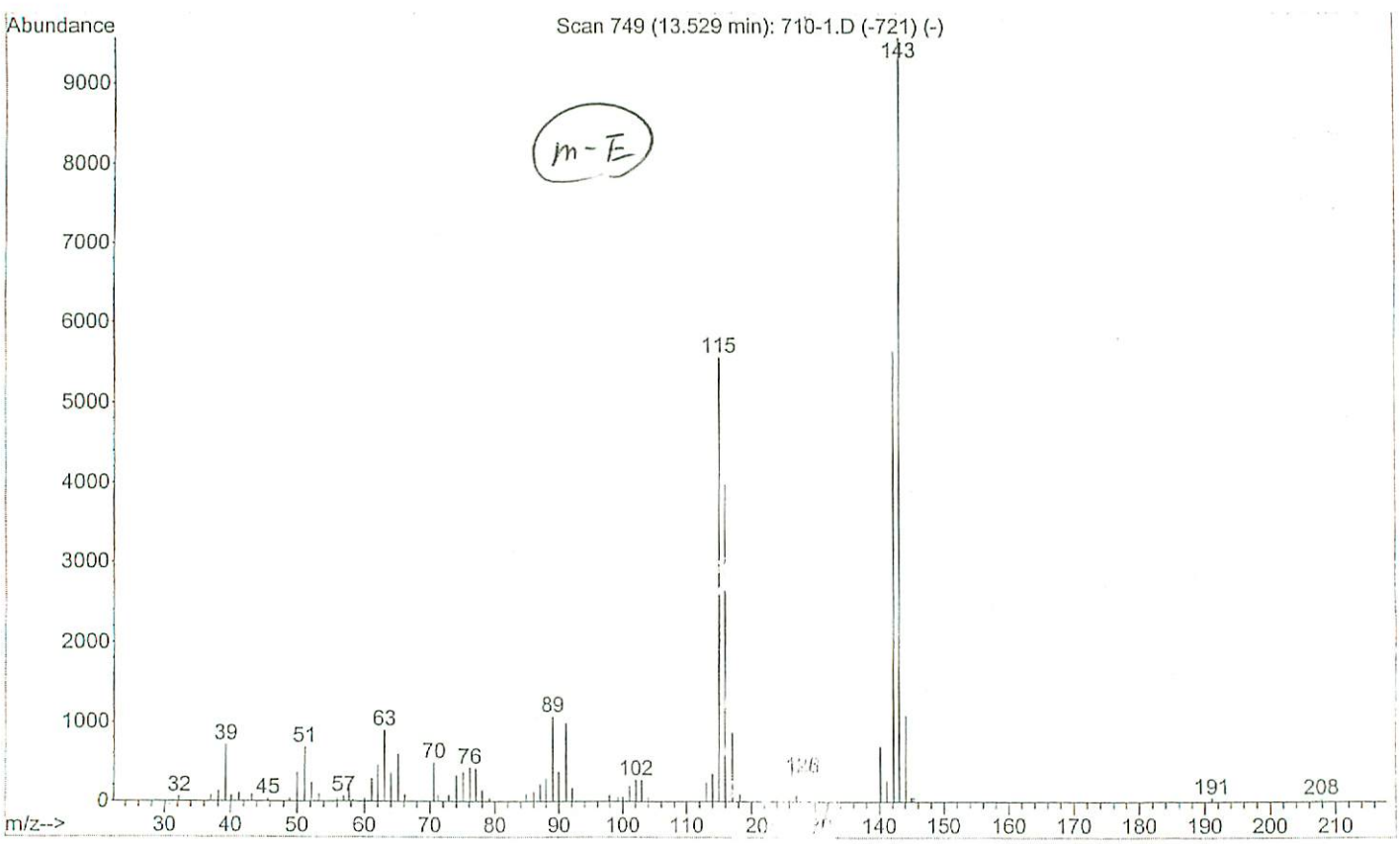
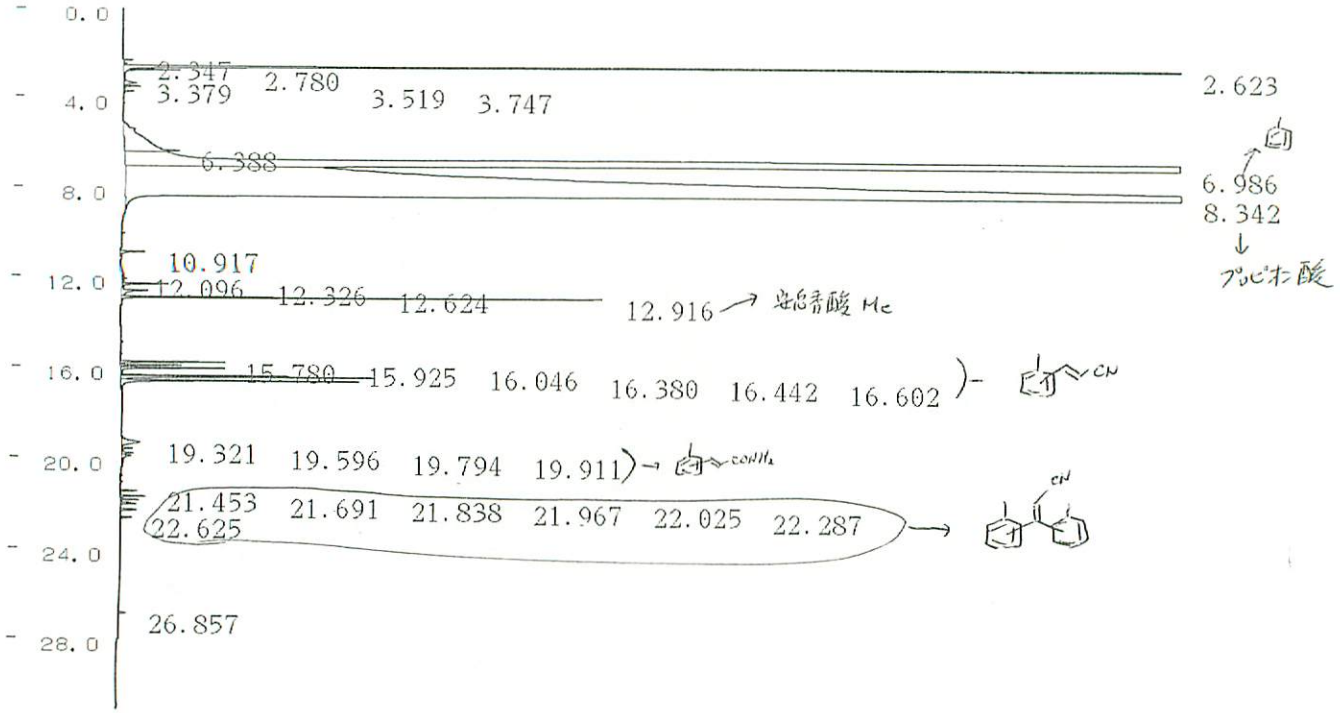

Abundance
Scan 749 (13.529 min): 710-1.D (-721) (-)
m-E
143
115
89
63
39
51
70
76
32
45
57
102
126
191
208
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
m/z--> 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

Table 2 entry 3 Toluene (120 mM), 5h.

CHROMATOPAC C-R7A CH=2 REPORT No.=1 ﾌｧｲﾙ=2:1221OK.C01 10/03/16 09:40:22



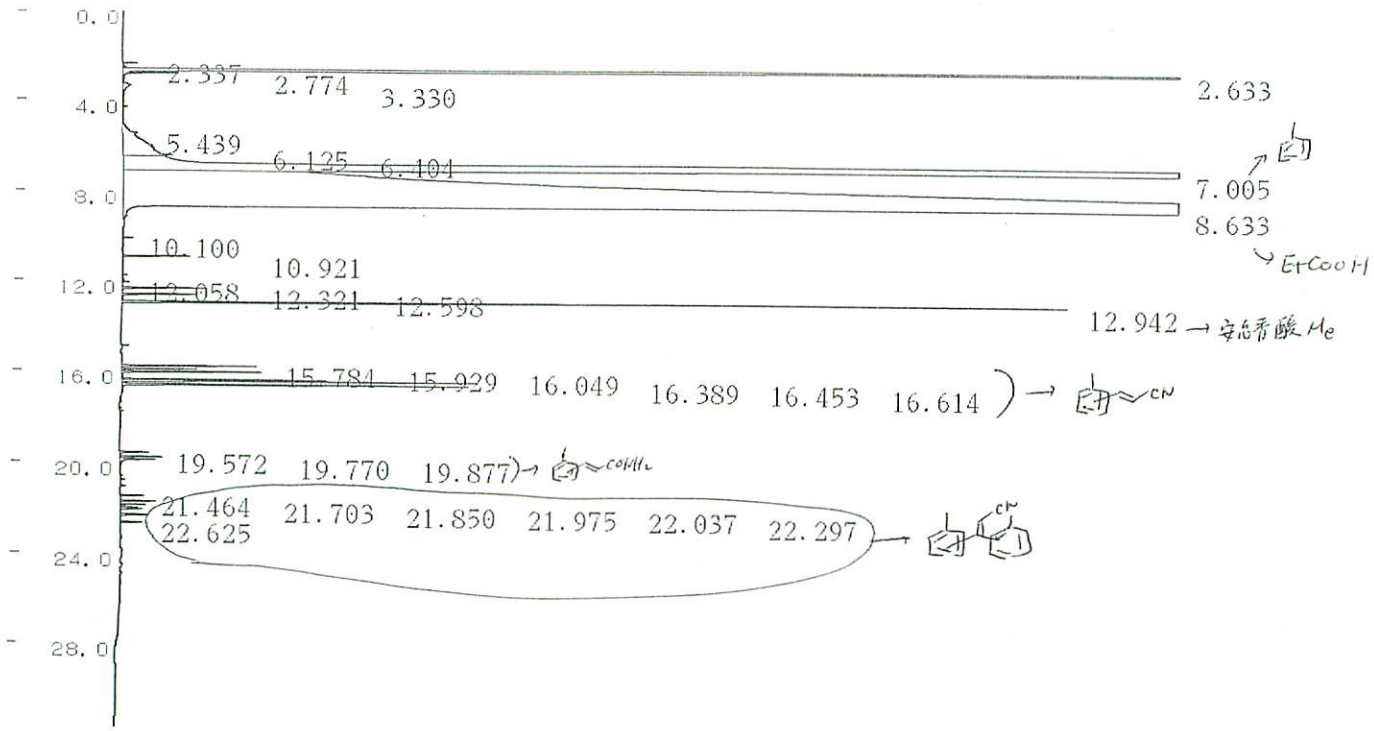
** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
2	1	2.347	1040	581			0.007	
	3	2.623	2214376	1175872	SV		14.863	
	4	2.78	5450	3070	T		0.0366	
	5	3.379	4965	712	T		0.0333	
	6	3.519	2502	939	TV		0.0168	
	7	3.747	1452	574	TV		0.0097	
	10	6.388	2127	828	T		0.0143	
	11	6.986	9170192	1100772	V		61.5506	
	12	8.342	3231250	105364	V		21.6882	
	15	10.917	5016	1441			0.0337	
	17	12.096	1906	262	V		0.0128	
	18	12.326	8453	2761	V		0.0567	
	19	12.624	8920	1557	V		0.0599	
	20	12.916	63012	28889	V		0.4229	
	22	15.78	14264	6?76			0.0957	
	23	15.925	8606	3021	V		0.0578	
	24	16.046	16030	6220	V		0.1076	
	25	16.38	22592	9966	V		0.1516	
	26	16.442	37187	15175	V		0.2496	
	27	16.602	38934	14177	V		0.2613	
	28	19.321	10968	1035			0.0736	
	29	19.596	1881	581			0.0126	
	30	19.794	2767	644	V		0.0186	
	31	19.911	3038	397	V		0.0204	
	35	21.453	2449				0.0164	
	36	21.691	3992	[illegible]	V		0.0268	
	37	21.838	2896	[illegible]	V		0.0194	
	38	21.967	1758	686	V		0.0118	
	39	22.025	2497	933	V		0.0168	
	40	22.287	4045	994	V		0.0272	
	41	22.625	2338	687	V		0.0157	
	42	26.857	1734	447			0.0116	
		TOTAL	14898617	2489103			100	

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

Table 2 entry 4 Toluene (90 mmol) 24h

CHROMATOPAC C-R7A CH=1 REPORT No.=6 クロマト=2:10610K.C01 09/08/04 16:23:38



** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.337	1522	859			0.0082	
	3	2.633	4611650	1875409	SV		24.8567	
	4	2.774	5340	3005	T		0.0288	
	6	3.33	5108	464	TV		0.0275	
	9	5.439	1102	283	T		0.0059	
	10	6.125	3825	69	T		0.0206	
	11	6.404	1766	623	T		0.0095	
	12	7.005	8283999	978462	V		44.6505	
	13	8.633	5254188	167376	SV		28.3199	
	15	10.1	1369	632			0.0074	
	17	10.921	8433	4079			0.0455	
	21	12.058	1234	456	V		0.0067	
	22	12.321	11434	5103	V		0.0616	
	24	12.598	10976	4461			0.0592	
	26	12.942	135948	57134	V		0.7328	
	33	15.784	17644	8038			0.0951	
	34	15.929	9622	4509	V		0.0519	
	35	16.049	18624	8311	V		0.1004	
	37	16.389	28543	12174			0.1538	
	38	16.453	468	21325	V		0.2525	
	39	16.614	48	20695	V		0.2603	
	45	19.572	4 1	1695			0.0236	
	46	19.77	3	2498			0.0354	
	47	19.877	3605	2083			0.0359	
	51	21.464	3388	1399			0.0183	
	52	21.703	357	2126	V		0.0289	
	3	21.85	3812	1487	V		0.0205	
		21.975	2597	1088	V		0.014	
		22.037	3252	1287	V		0.0175	
	56	22.297	6034	1588			0.0325	
	57	22.625	3497	1271			0.0188	
			3189904				100	

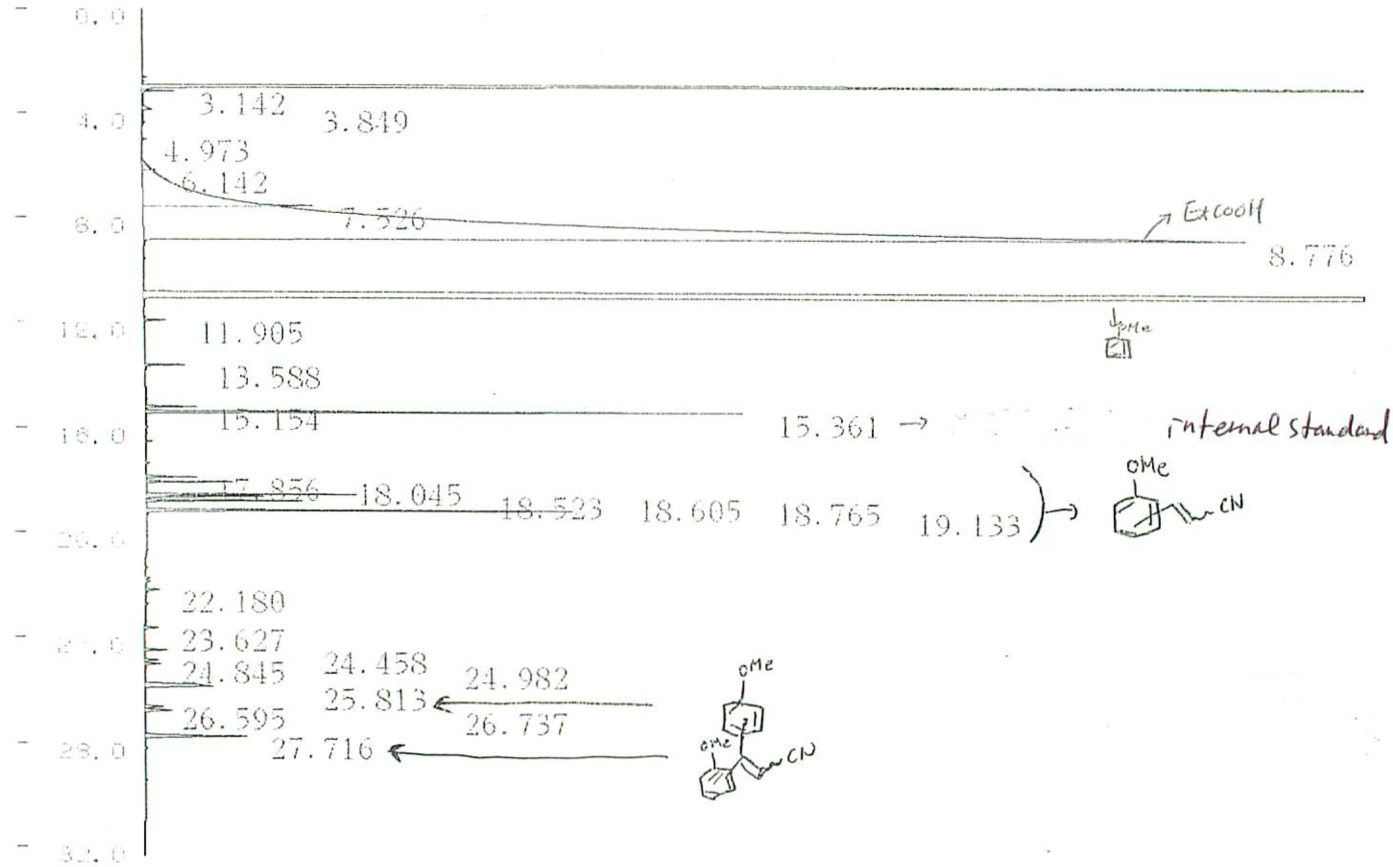
106

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

Table 2

entry 5.

CHROMATOPAC C-R7A CH=1 REPORT No.=16 [illegible]=2:7140KA.C00 08/09/11 18:49



** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	3	2.96	2429186	1136066	V		31.4837	
	4	3.142	2779	1486	L		0.036	
	5	3.849	3142	519	L		0.0407	
	7	4.973	3691	227	V		0.0478	
	8	6.142	8180	703			0.106	
	9	7.526	241356	8799	V		3.1281	
	10	8.776	1792676	57566	V		23.2342	
	12	11.009	2915137	427477			37.7819	
	15	11.905	3272	1124	V		0.0424	
	17	13.588	5310	2047			0.0688	
	20	15.154	7195	2758			0.0933	
	21	15.361	80986	31275	V		1.0496	
	27	17.856	7537	2661 m-Z			m-Z 0.0977	
	28	18.045	11132	4507 o-Z			o-Z 0.1443	
	29	18.523	28542	10938 p-Z			p-Z [illegible]	
	30	18.605	15464	6119 m-E			m-E [illegible]	
	31	18.765	21050	8092 o-E			o-E [illegible]	
	32	19.133	65857	22195 p-E			p-E [illegible]	
	39	22.18	3083	706			[illegible]	
	44	23.627	2608	673	V		[illegible]	
	45	24.458	3980	1147			[illegible]	
	46	24.8[illegible]	2453	683			[illegible]	
	47	24.98[illegible]	2939	817	V		[illegible]	
	[illegible]	25.813	24171	3502			[illegible]	
	[illegible]	26.595	3800	930			[illegible]	
	5[illegible]	26.737	5847	1427	V		0.0758	
	5[illegible]	27.716	24322	5258	V		0.3152	

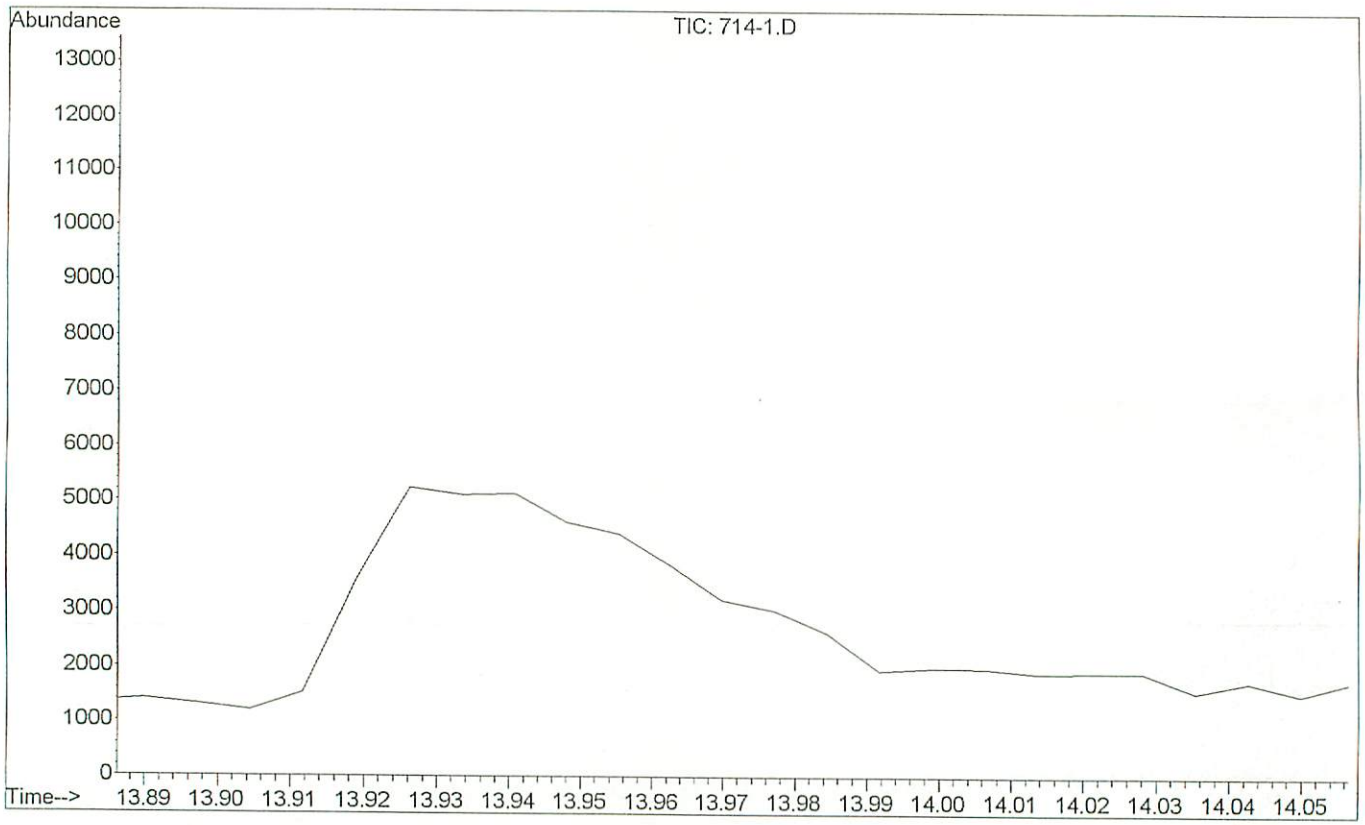
o m p
(66:34) 15 (67:33) 13 (70:30)

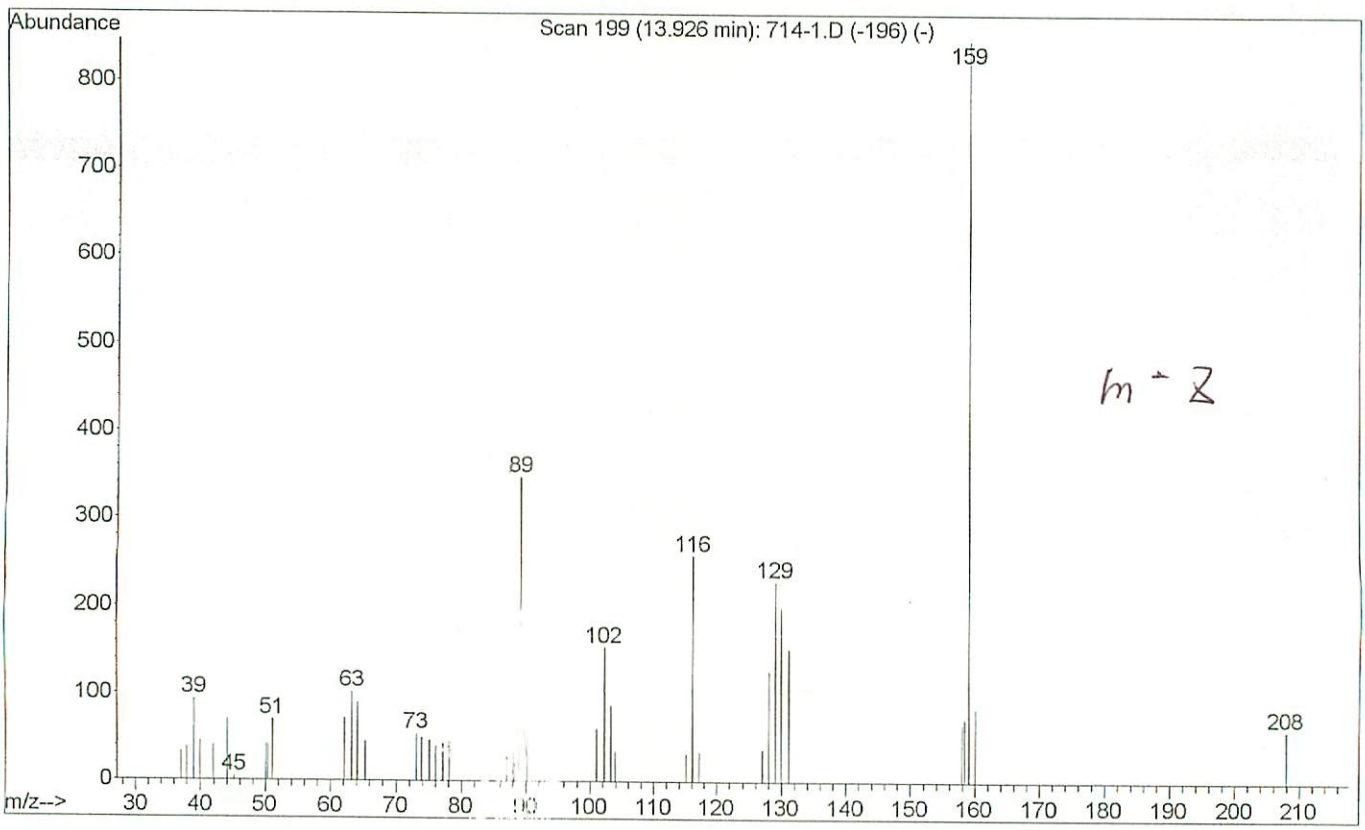
E/Z

69 : 31

This journal is (c) The Royal Society of Chemistry 2010

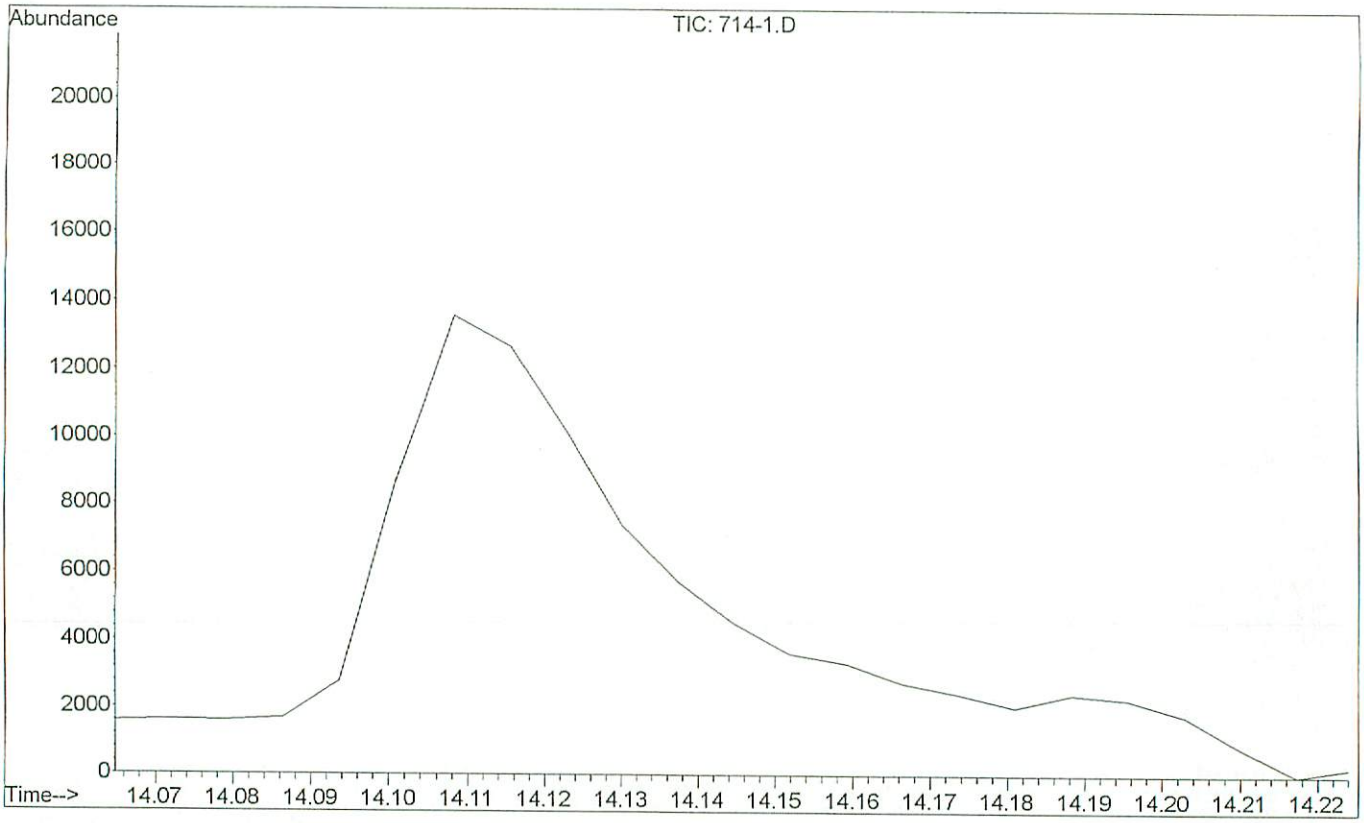
File : D:\FINE DATA\OKABE\714-1.D
Operator :
Acquired : 12 Sep 2008 9:29 using AcqMethod OKABE
Instrument : Instrumen
Sample Name: 714-1
Misc Info :
Vial Number: 14

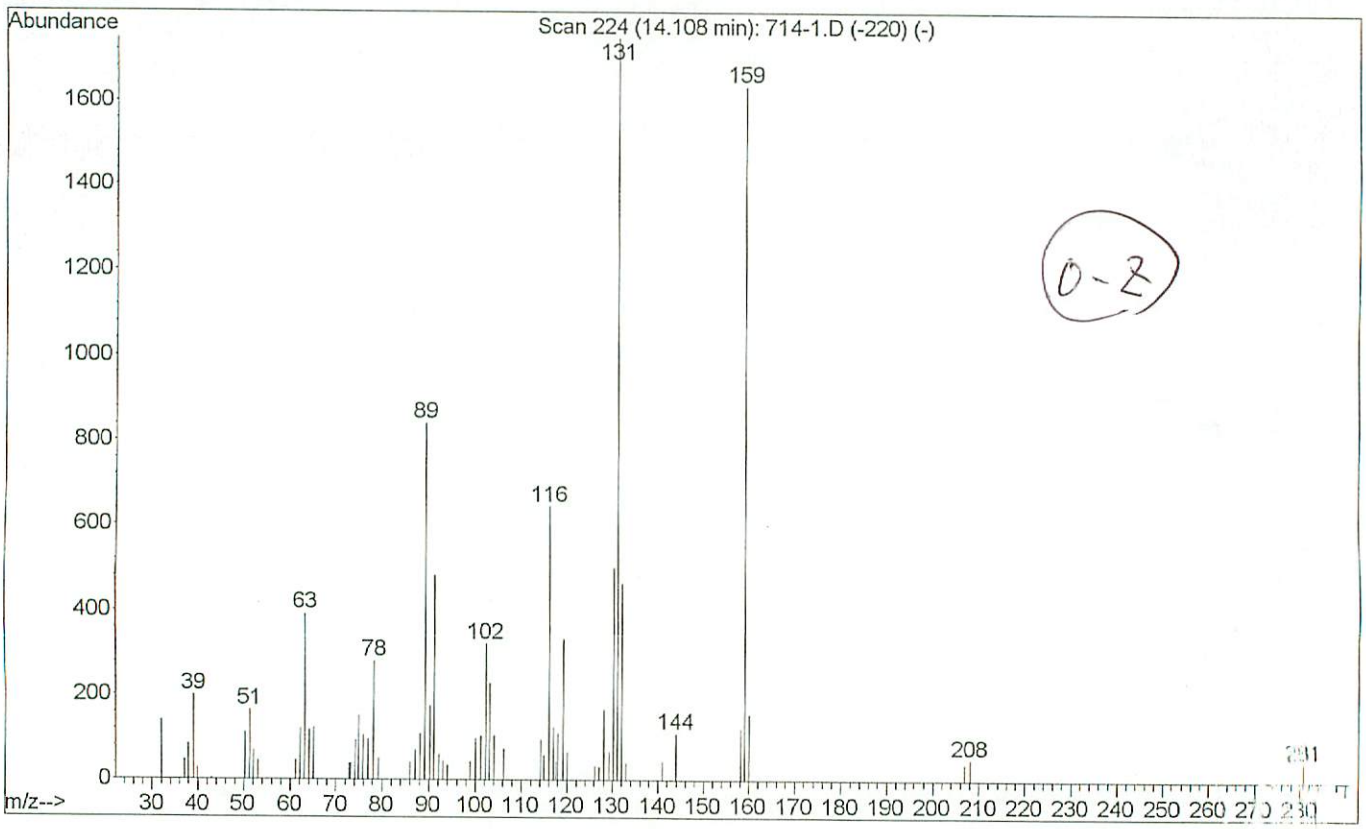




m - 2

File : D:\FINE DATA\OKABE\714-1.D
Operator :
Acquired : 12 Sep 2008 9:29 using AcqMethod OKABE
Instrument : Instrumen
Sample Name: 714-1
Misc Info :
Vial Number: 14



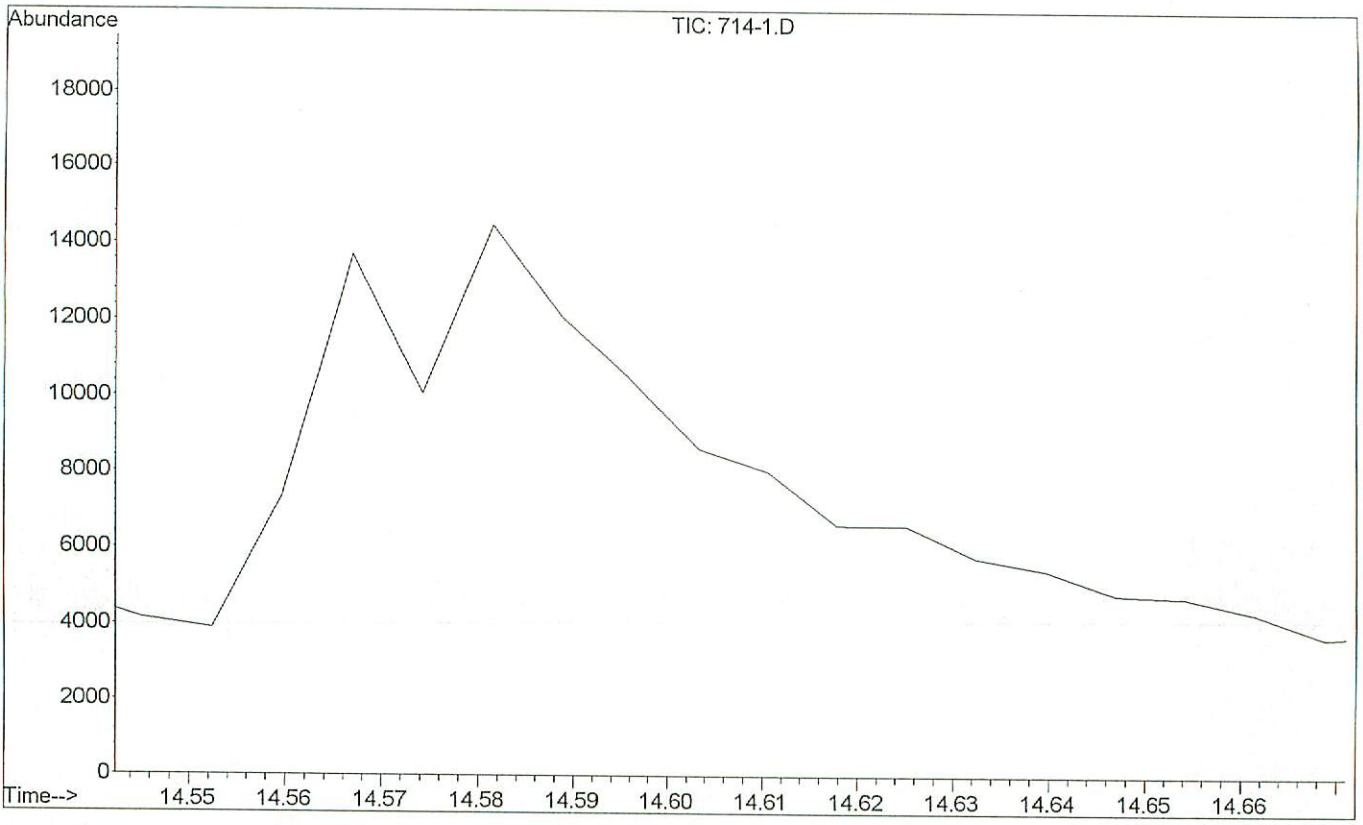


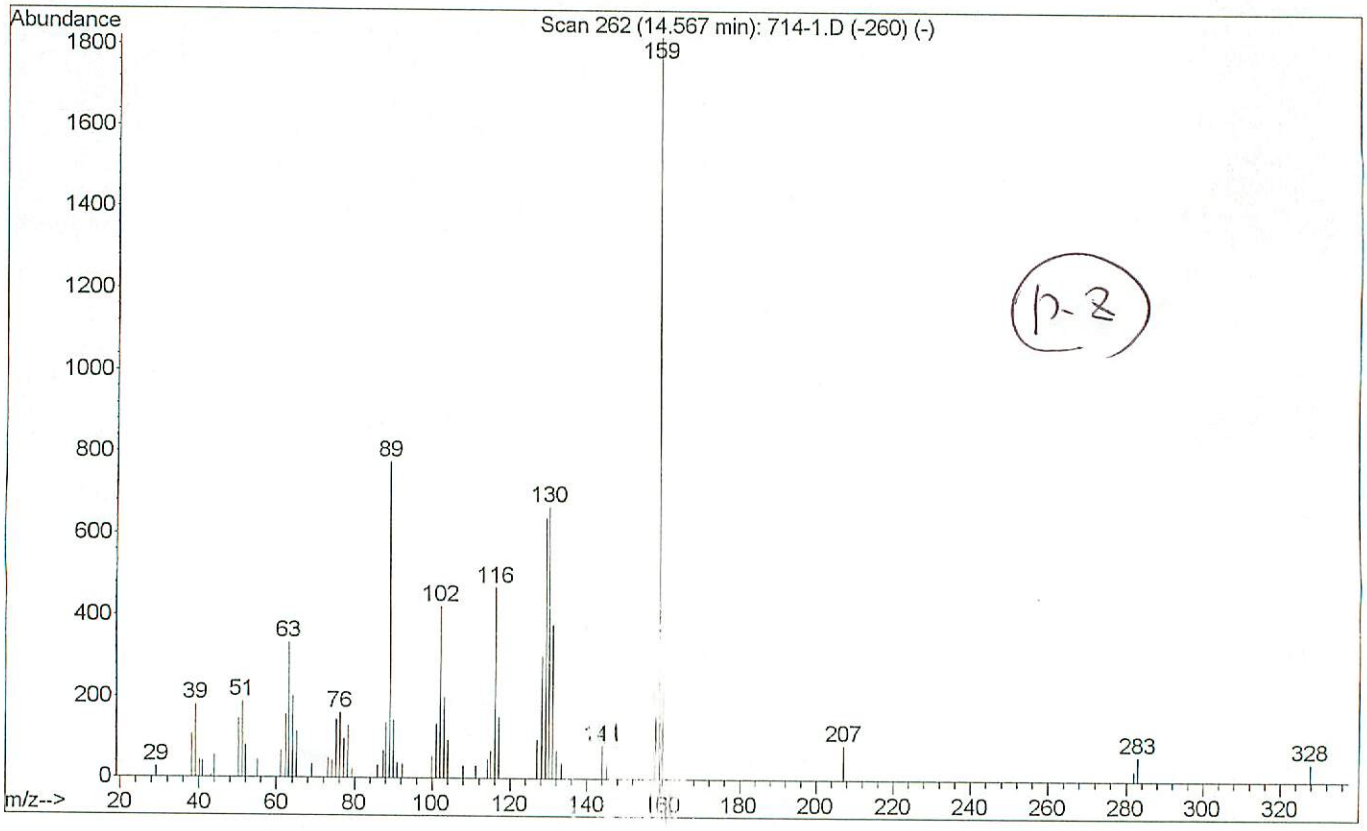
O-2

ok

This journal is (c) The Royal Society of Chemistry 2010

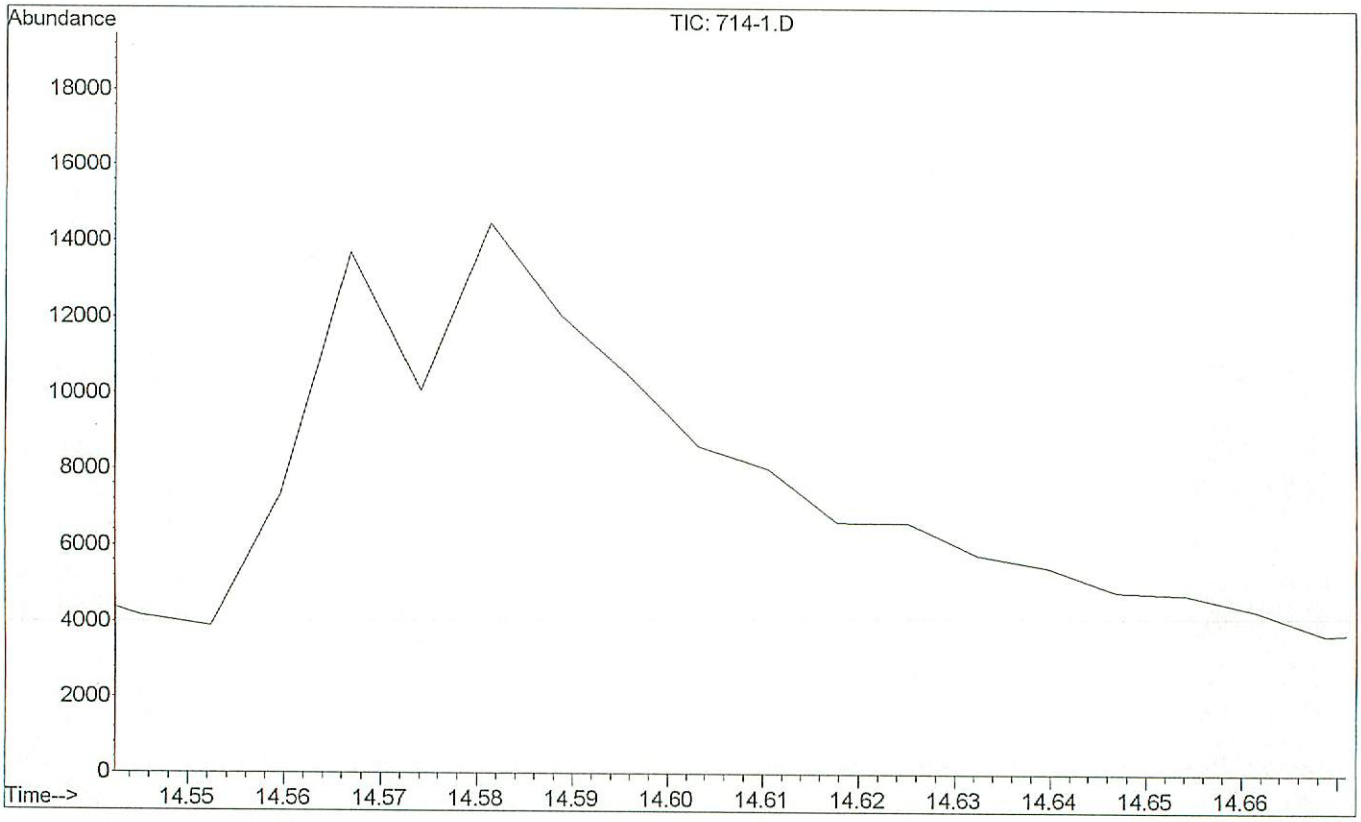
File : D:\FINE DATA\OKABE\714-1.D
Operator :
Acquired : 12 Sep 2008 9:29 using AcqMethod OKABE
Instrument : Instrumen
Sample Name: 714-1
Misc Info :
Vial Number: 14

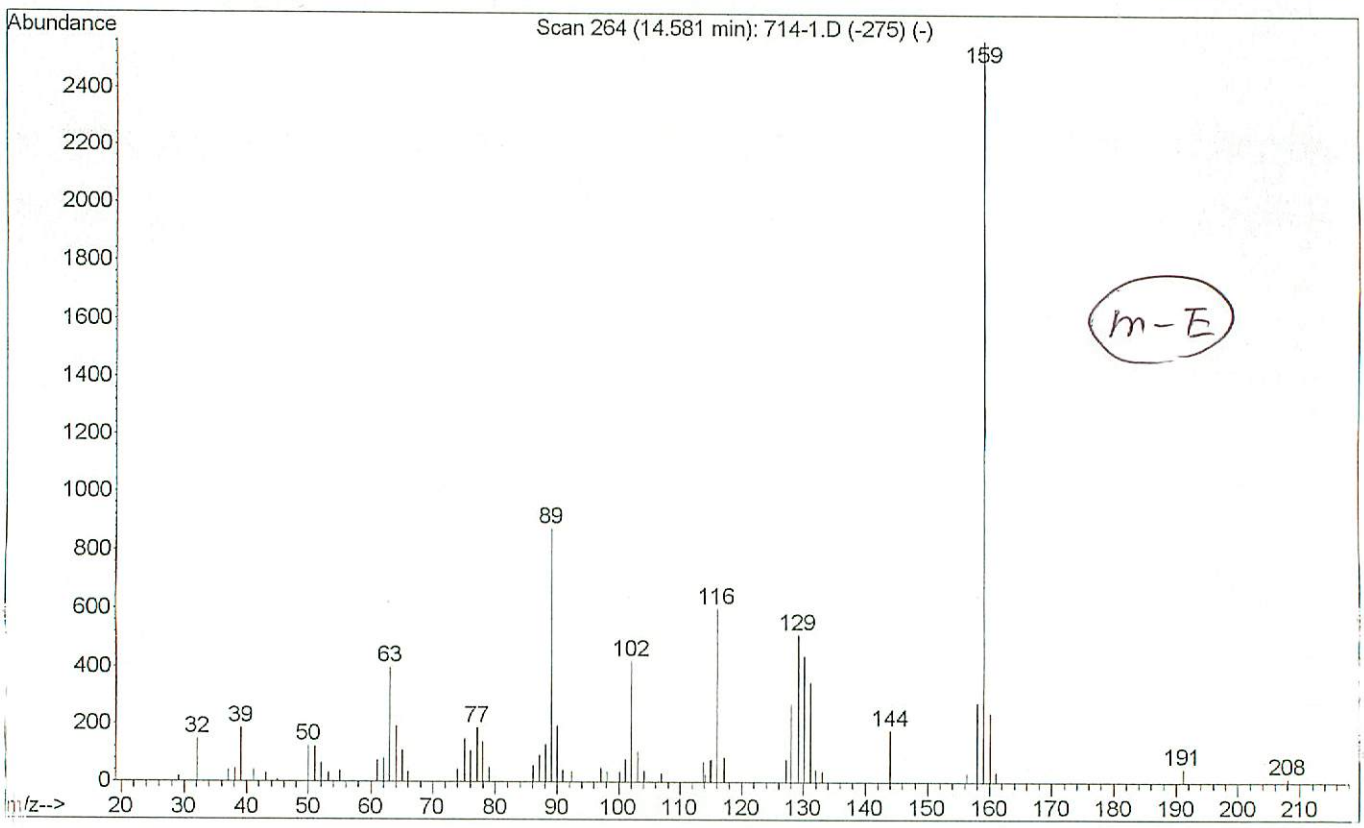




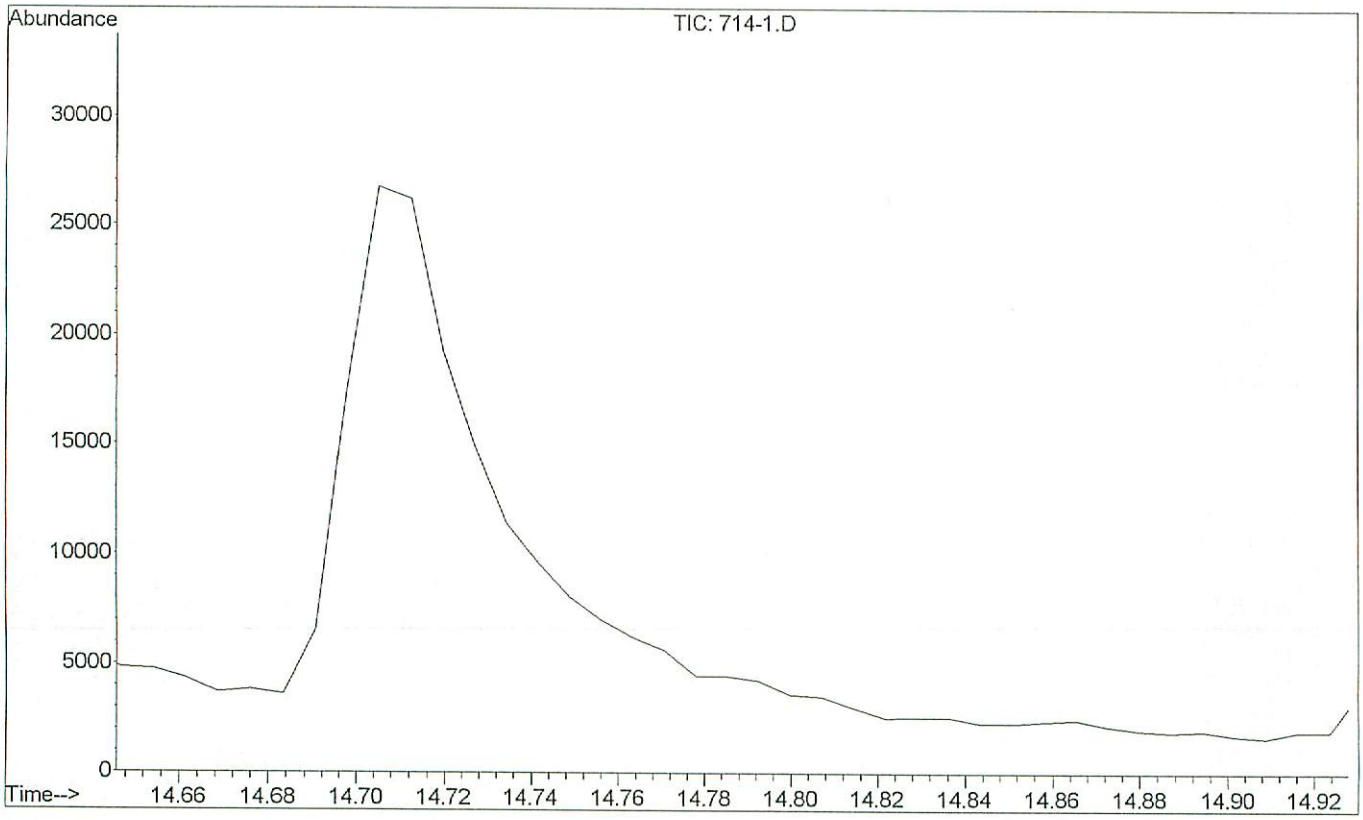
(p-2)

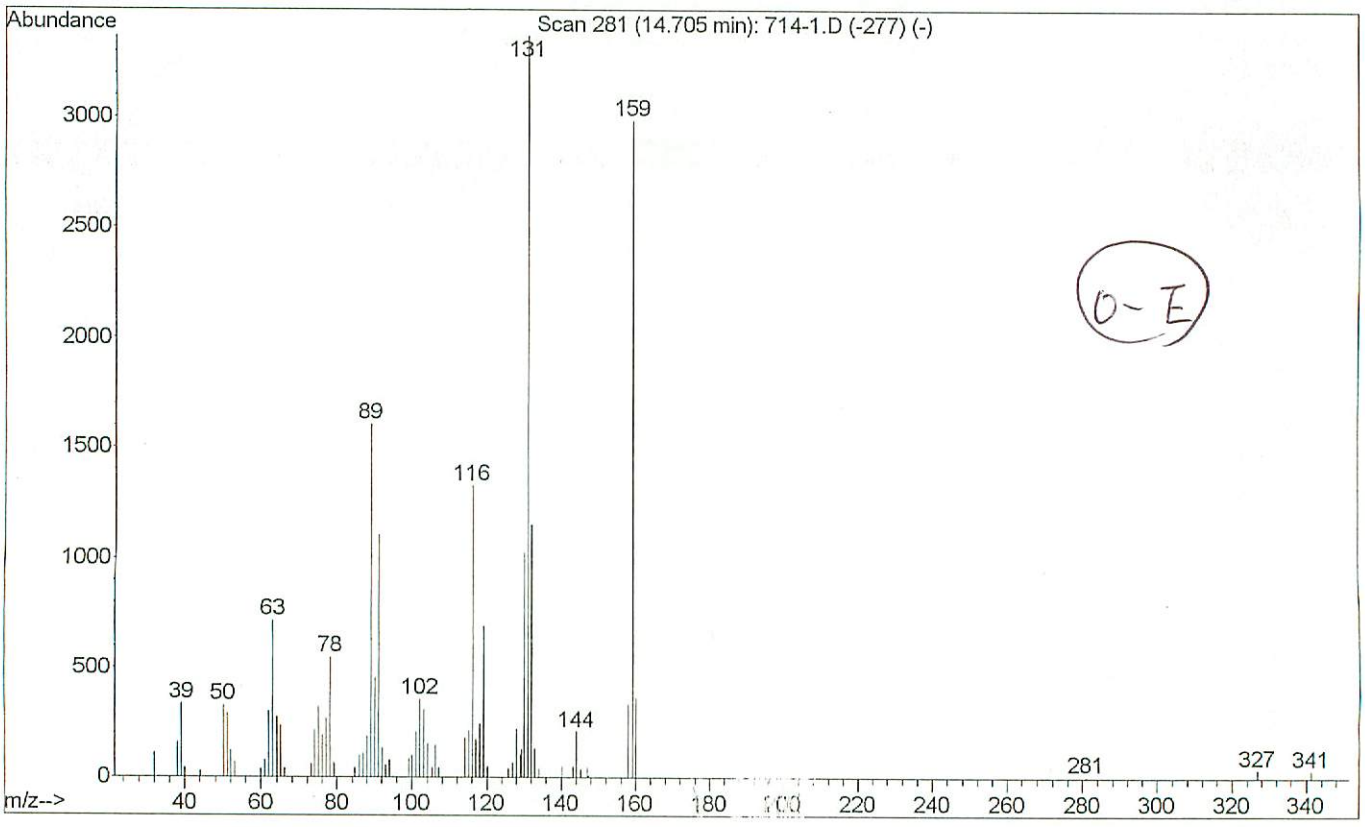
```
File        : D:\FINE DATA\OKABE\714-1.D
Operator    :
Acquired    : 12 Sep 2008    9:29      using AcqMethod OKABE
Instrument  :    Instrumen
Sample Name: 714-1
Misc Info   :
Vial Number: 14
```





File : D:\FINE DATA\OKABE\714-1.D
Operator :
Acquired : 12 Sep 2008 9:29 using AcqMethod OKABE
Instrument : Instrumen
Sample Name: 714-1
Misc Info :
Vial Number: 14

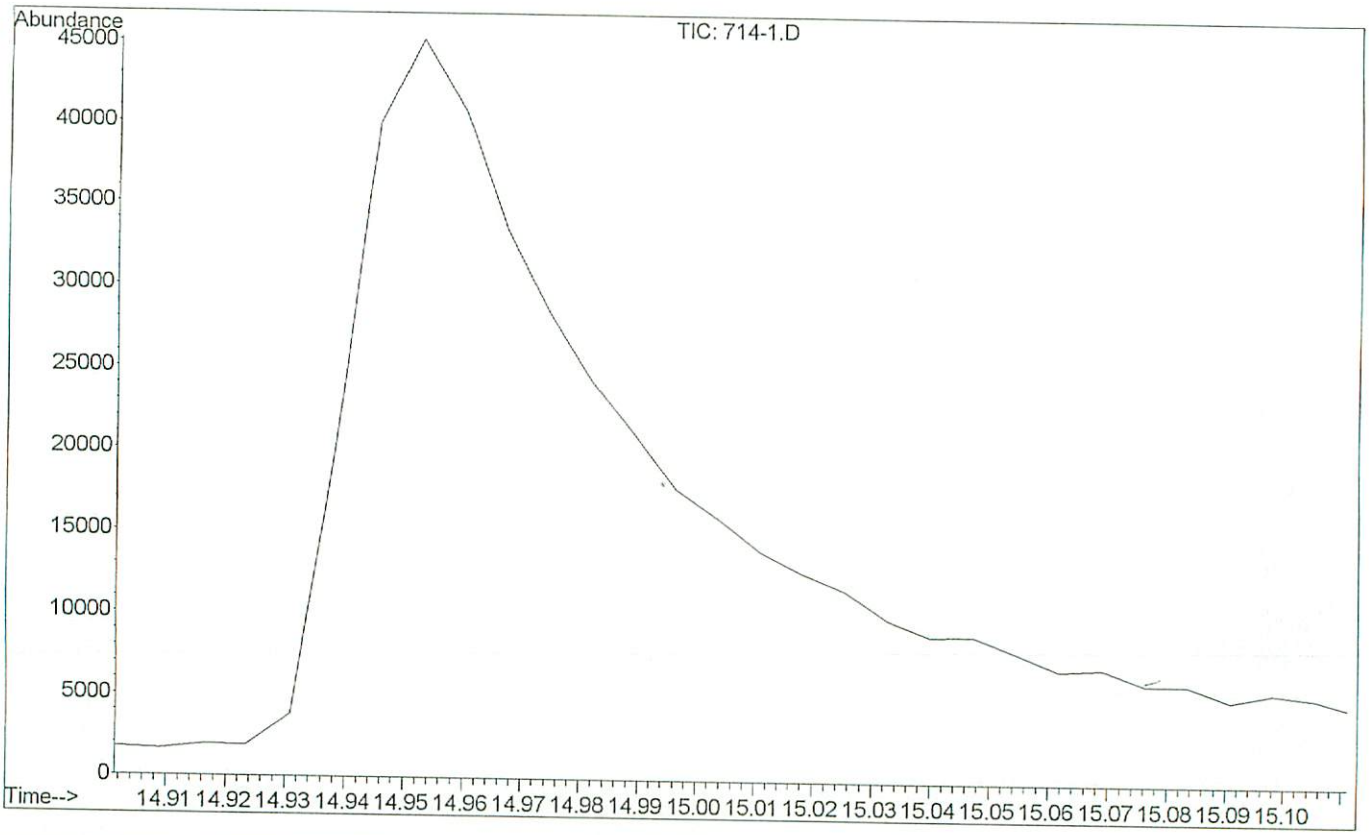


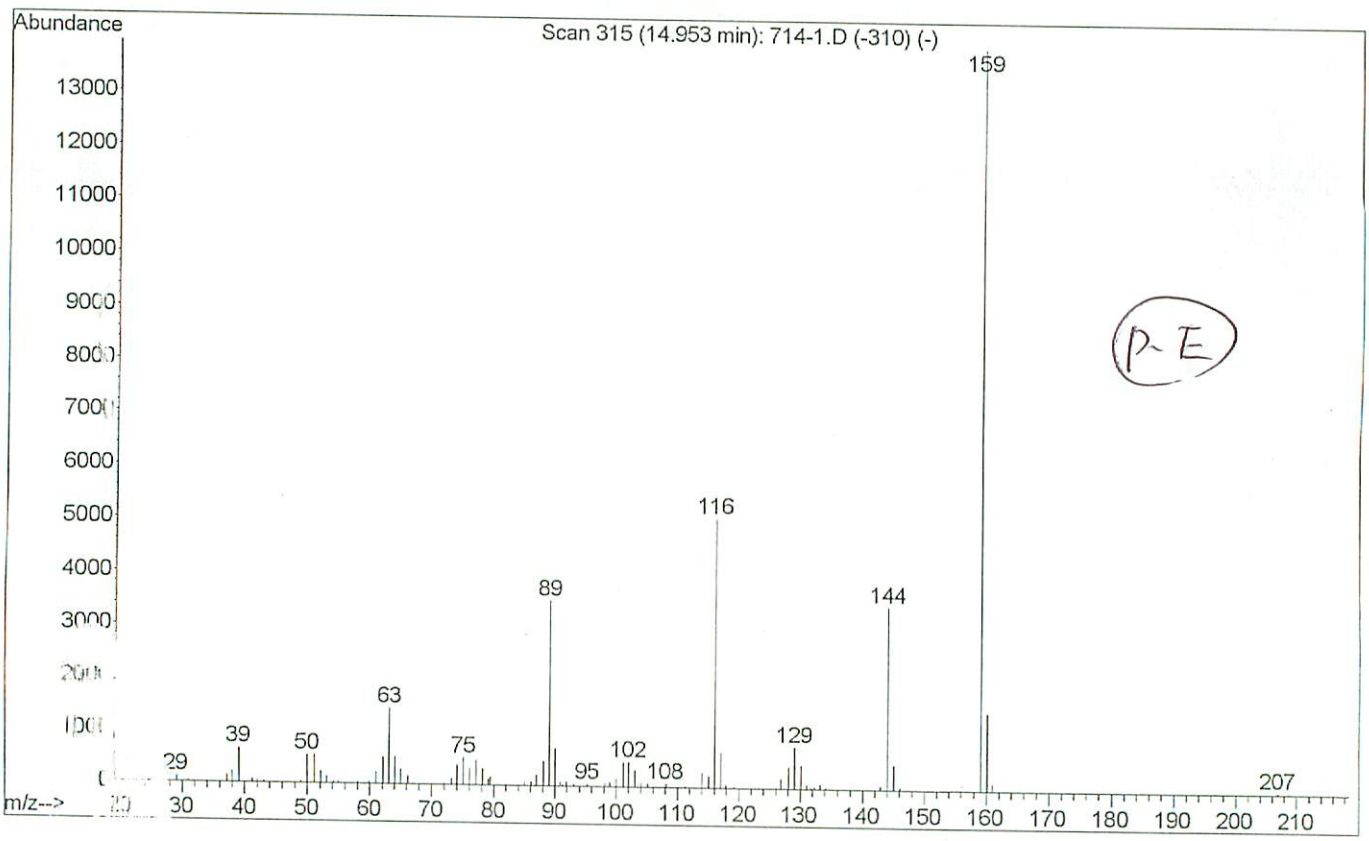


O-E

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

File : D:\FINE DATA\OKABE\714-1.D
Operator :
Acquired : 12 Sep 2008 9:29 using AcqMethod OKABE
Instrument : Instrumen
Sample Name: 714-1
Misc Info :
Vial Number: 14

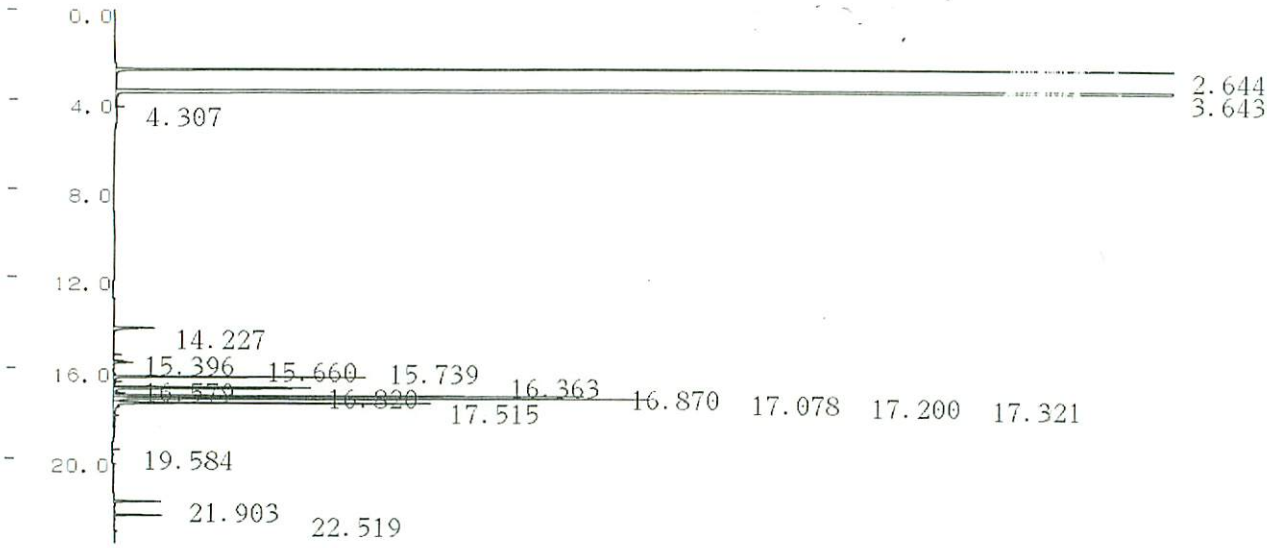


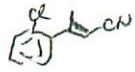


(P-E)

Table 2 entry 6

CHROMATOPAC C-R7A CH=1 REPORT No.=8 ｸﾛﾏﾄ=2:1225OK.C04 10/03/1[illegible] 17:54:52

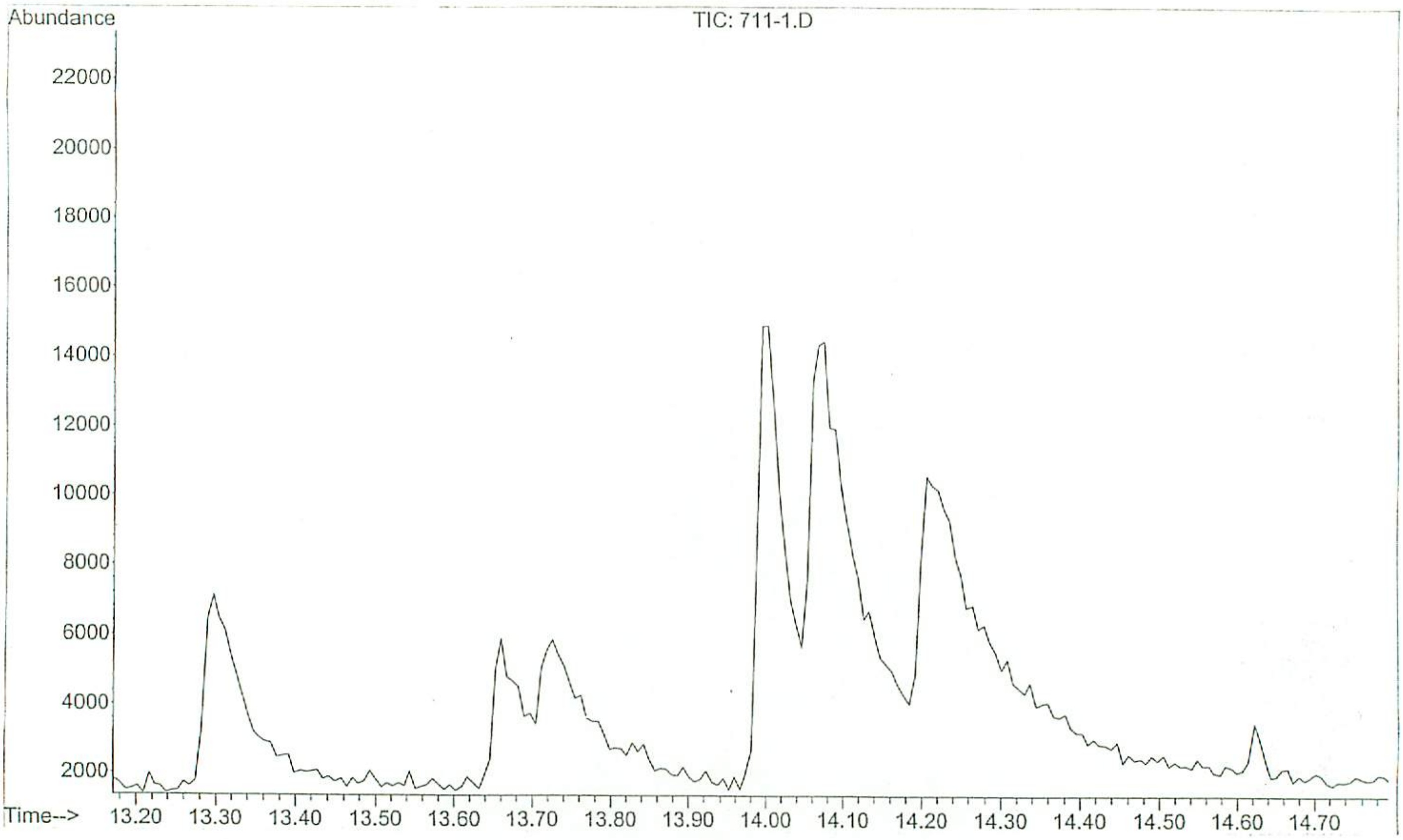


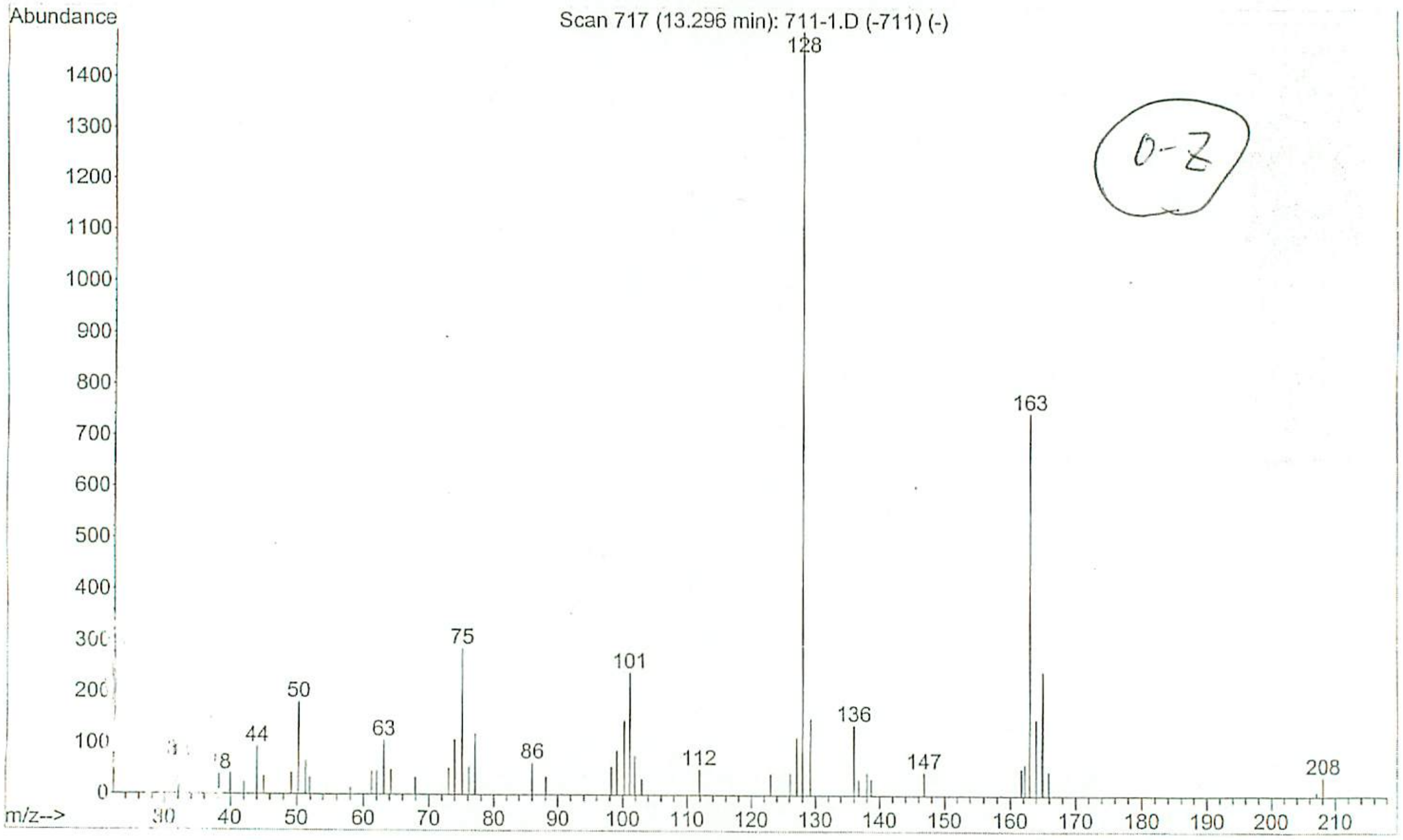


** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.644	583129	301678			19.2795	
	2	3.643	2118821	584716	L		70.0529	
	3	4.307	1534	419	V		0.0507	
	5	14.227	10403	2431			0.3439	
	6	15.396	1061	463			0.0351	
	7	15.66	1237	571			0.0409	
	8	15.739	3133	1154	V		0.1036	
	11	16.363	34138	14992	V		1.1287	→ o→Z
	12	16.579	1316	503	V		0.0435	—
	14	16.82	26209	11750	V		0.8665	→ p→Z
	15	16.87	24558	10654	V		0.812	→ m→Z
	16	17.078	1984	667	V		0.0656	
	17	17.2	69017	28217	V		2.2819	→ o→E
	18	17.321	80823	32060	V		2.6722	→ p→E
	19	17.515	51962	18947	SV		1.718	→ m→E
	25	19.584	1007	450			0.0333	
	31	21.903	7419	2811	V		0.2453	
	35	22.519	6851	2822	V		0.2265	
		TOTAL	3024600	1015303			100	

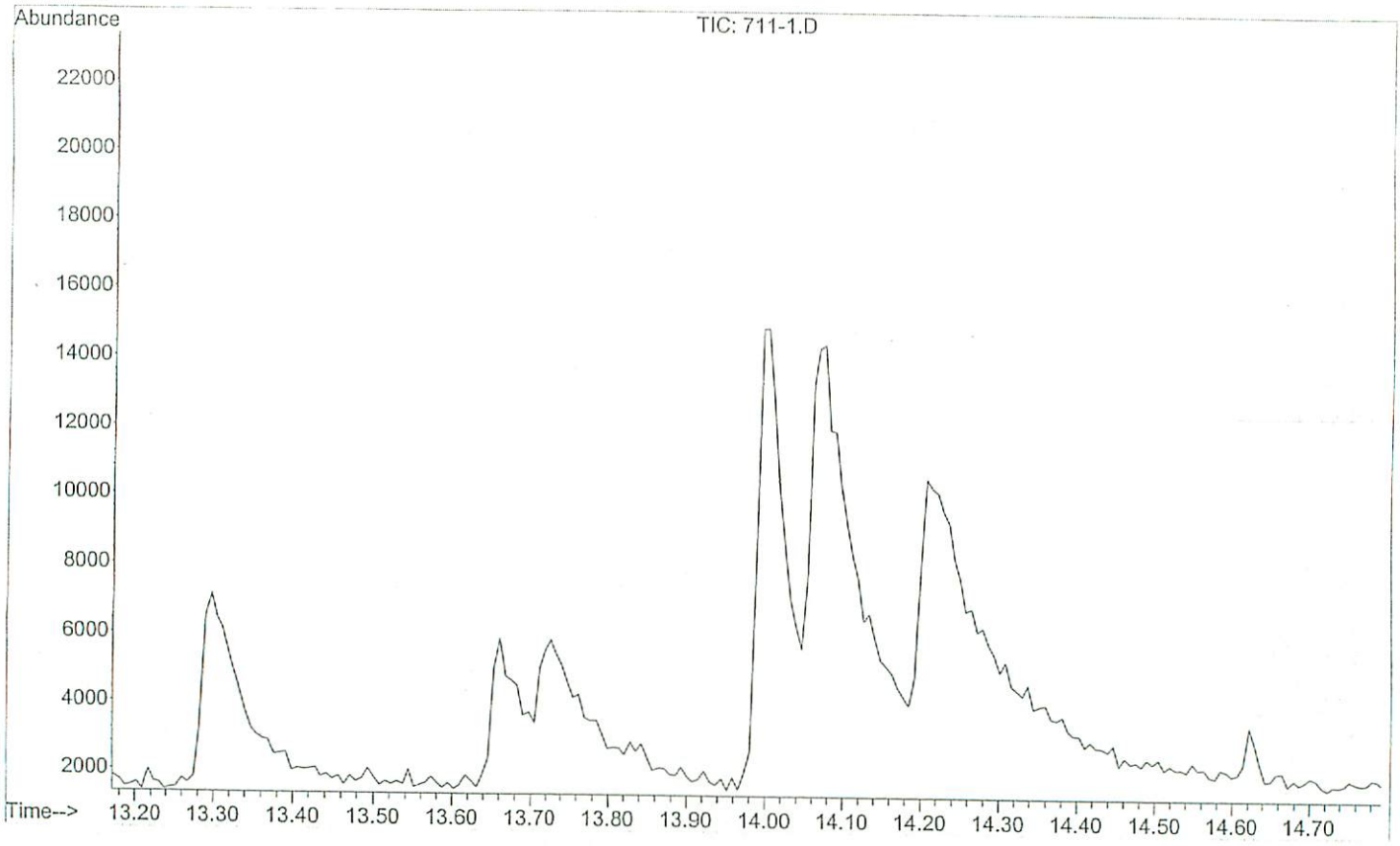
28,67o7

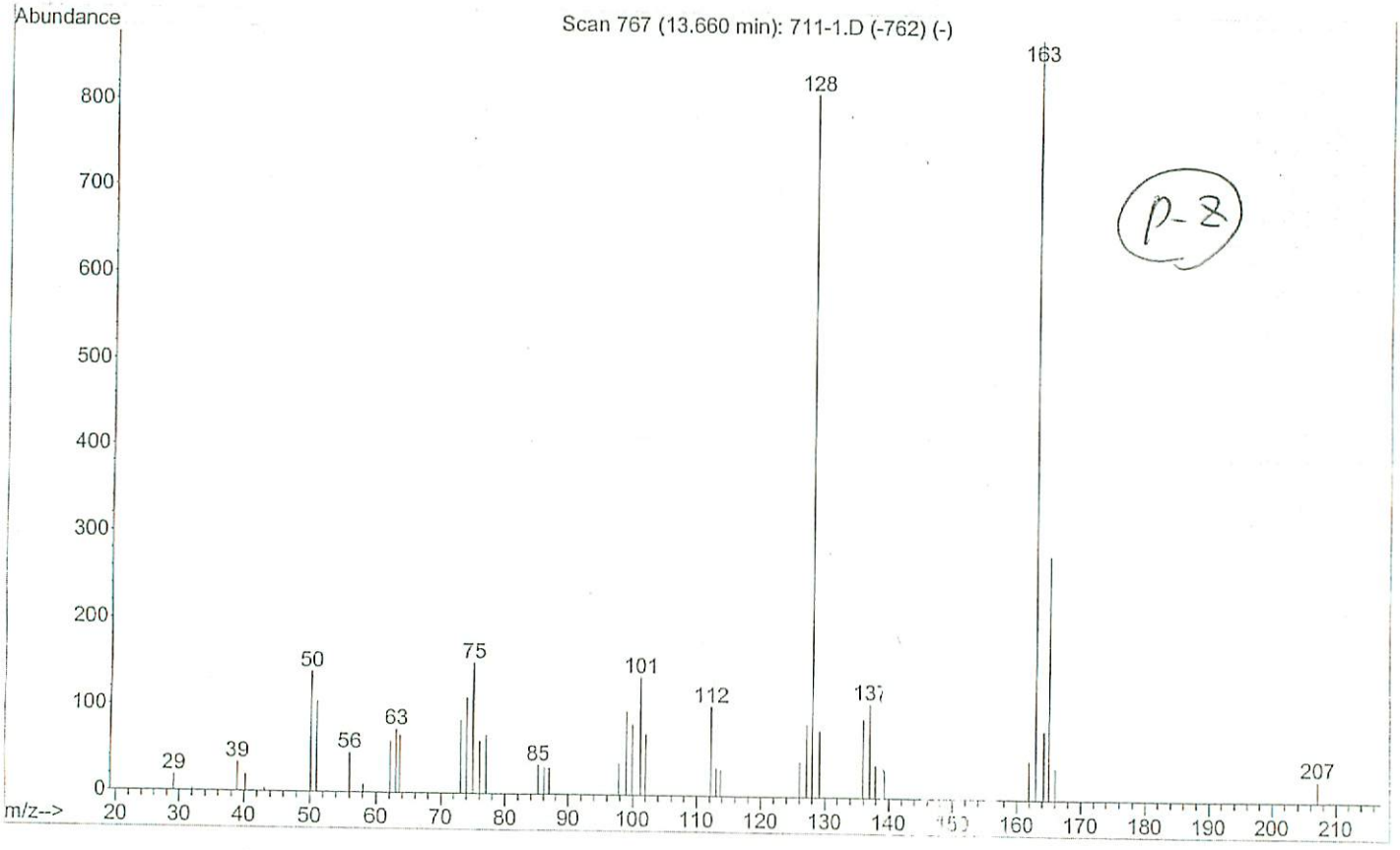

Abundance
TIC: 711-1.D
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
Time-->
13.20 13.30 13.40 13.50 13.60 13.70 13.80 13.90 14.00 14.10 14.20 14.30 14.40 14.50 14.60 14.70


Abundance
Scan 717 (13.296 min): 711-1.D (-711) (-)
128
O-Z
163
75
101
50
136
63
44
86
112
147
208
1400
1300
1200
1100
1000
900
800
700
600
500
400
100
0
m/z-->
40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

0 体

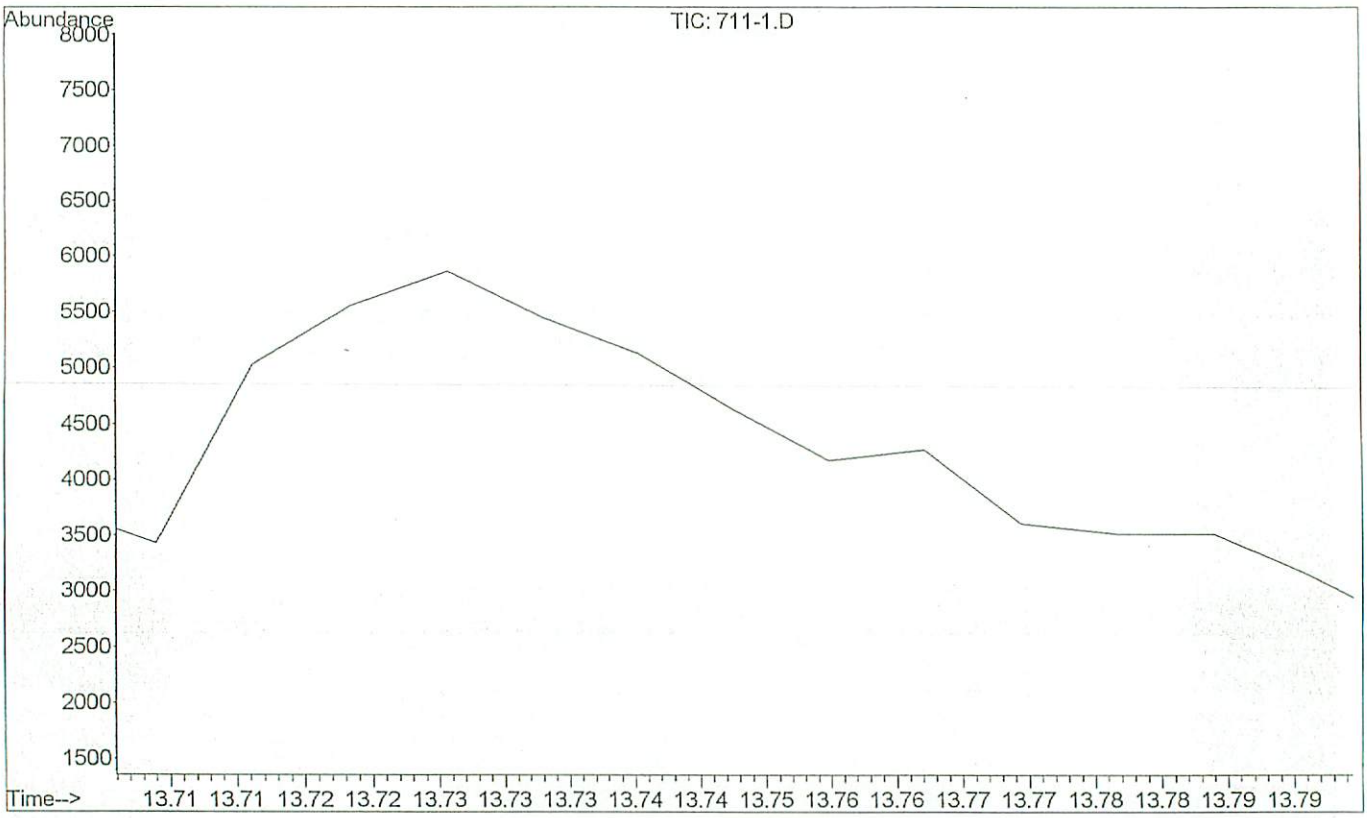
This journal is (c) The Royal Society of Chemistry 2010

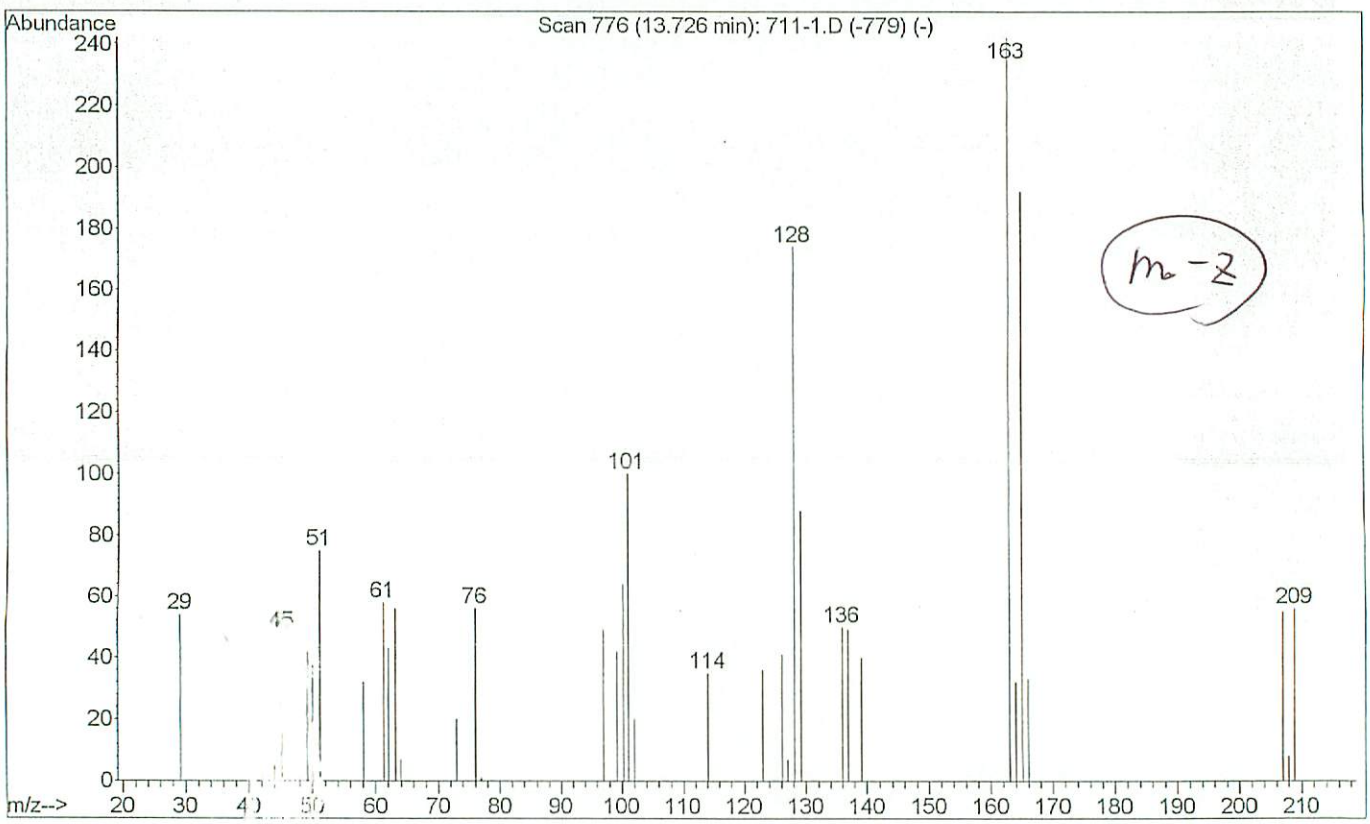




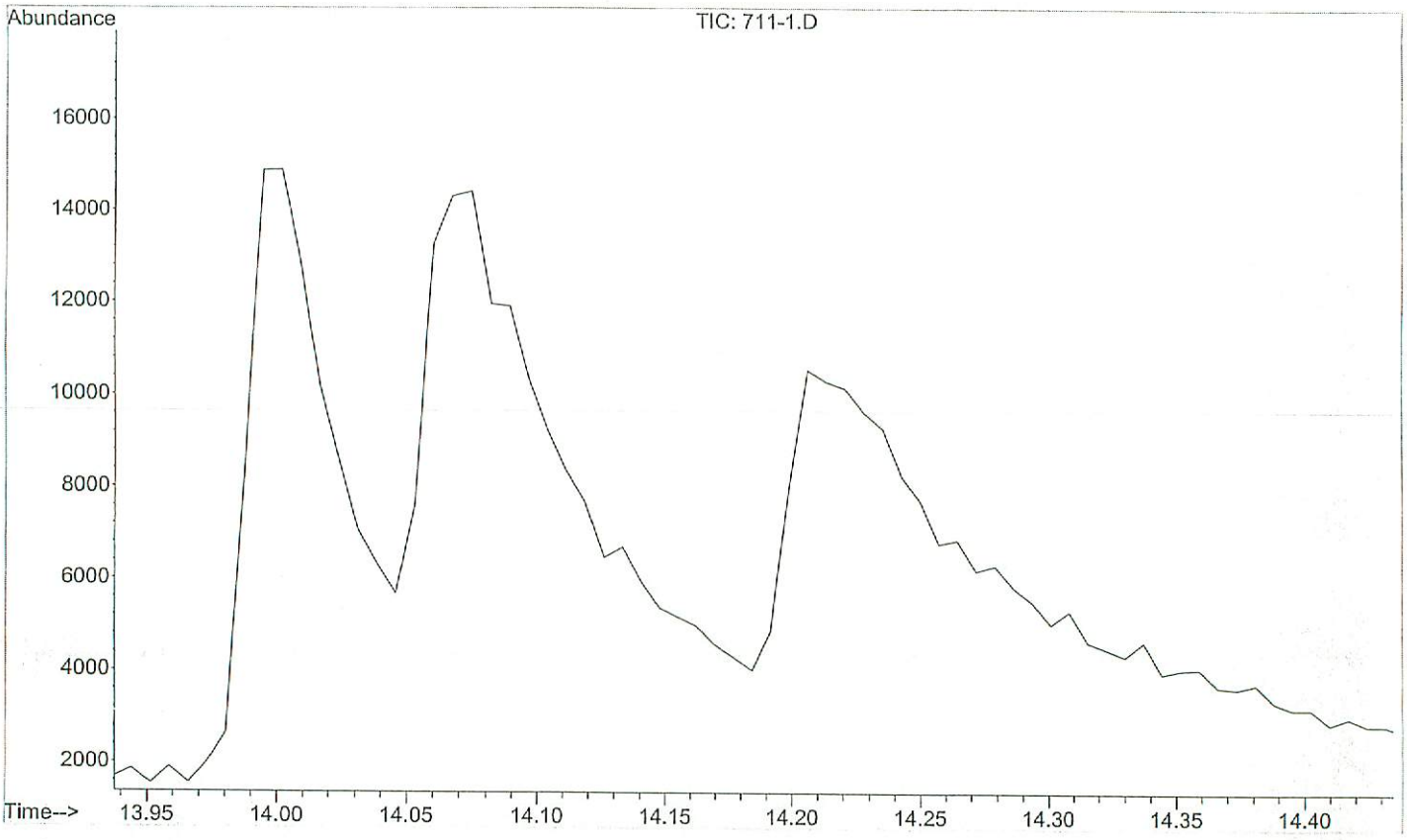
This journal is (c) The Royal Society of Chemistry 2010

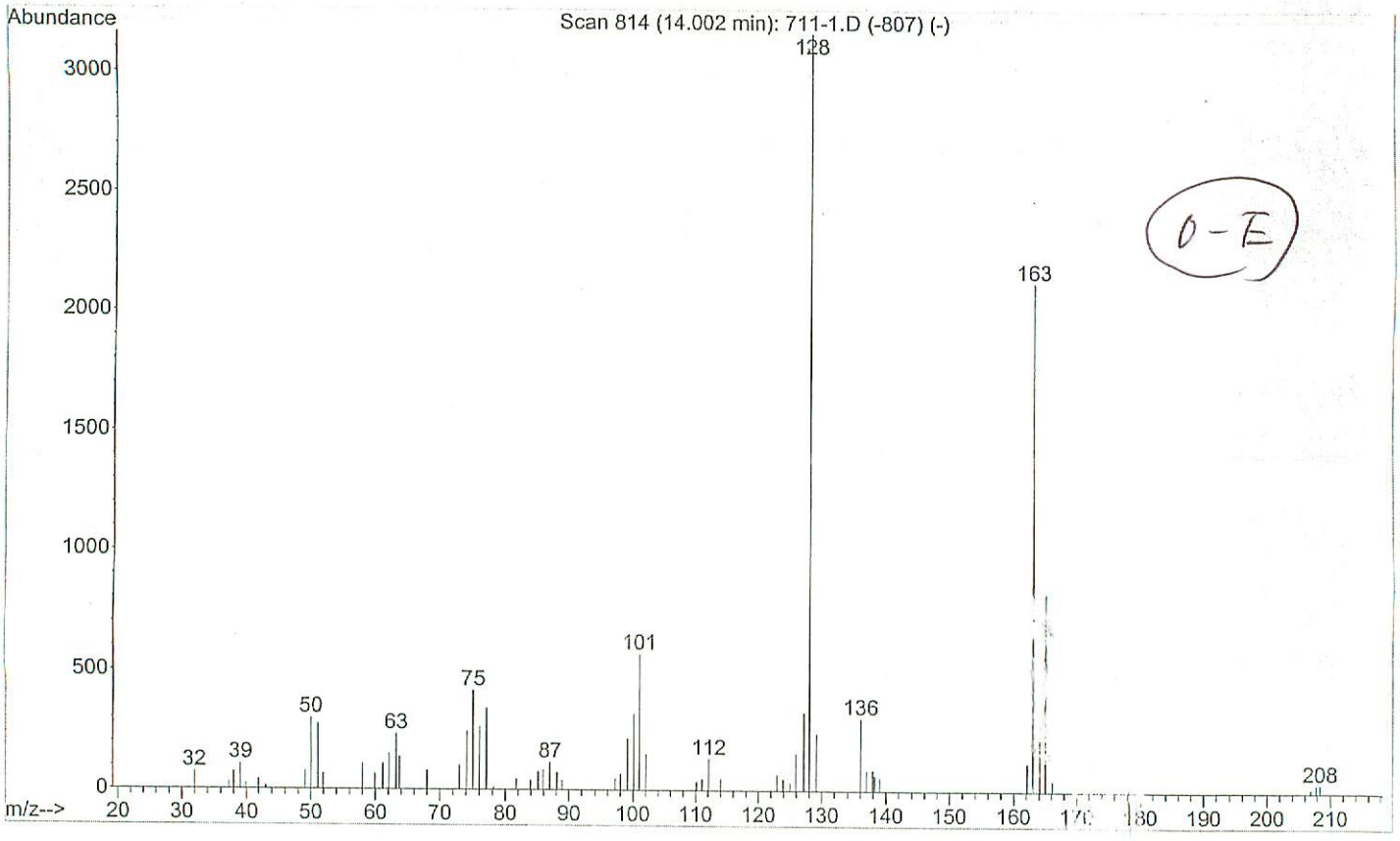
```
File        : D:\FINE DATA\OKABE\711-1.D
Operator    :
Acquired    :  9 Sep 2008  21:29      using AcqMethod OKABE
Instrument  :    Instrumen
Sample Name: 711-1
Misc Info   :
Vial Number: 11
```





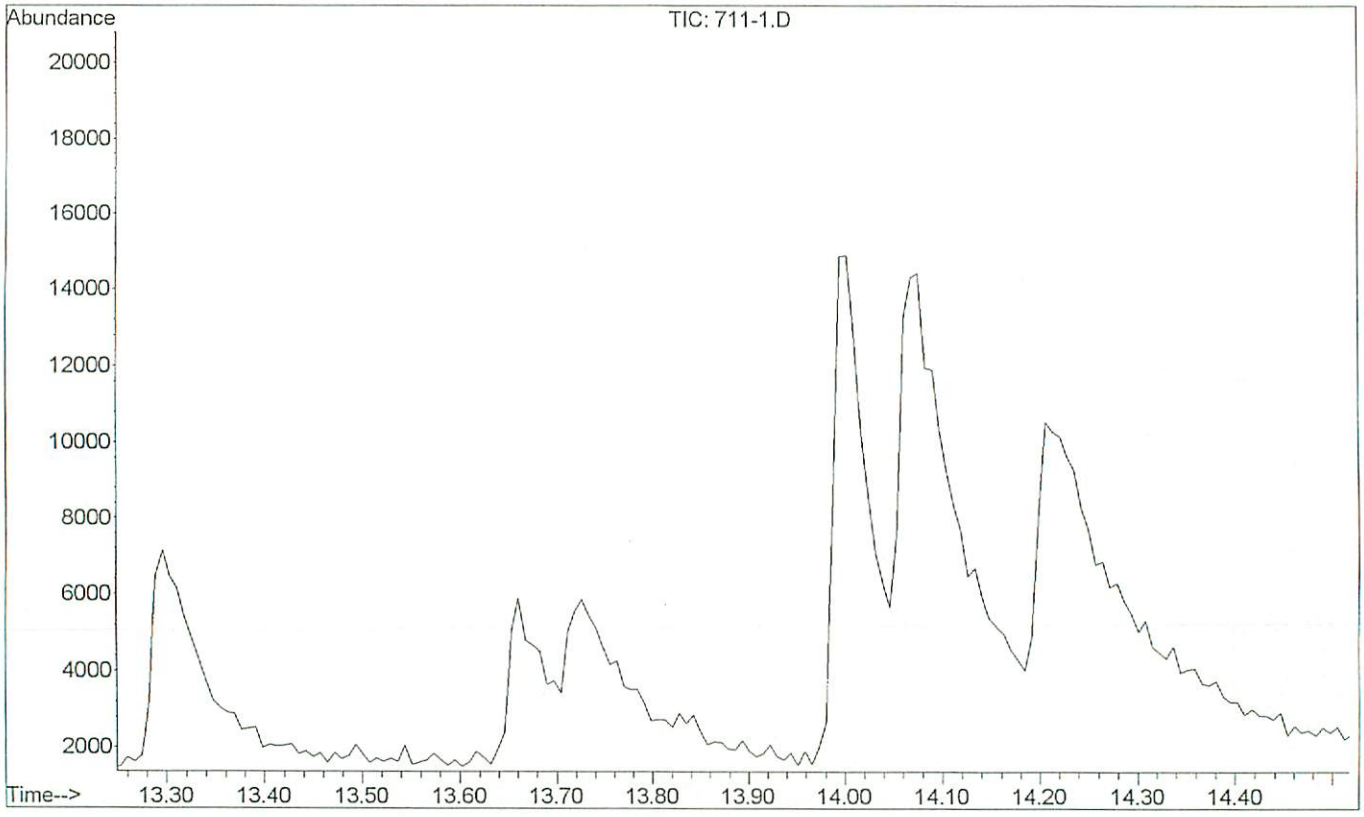
This journal is (c) The Royal Society of Chemistry 2010

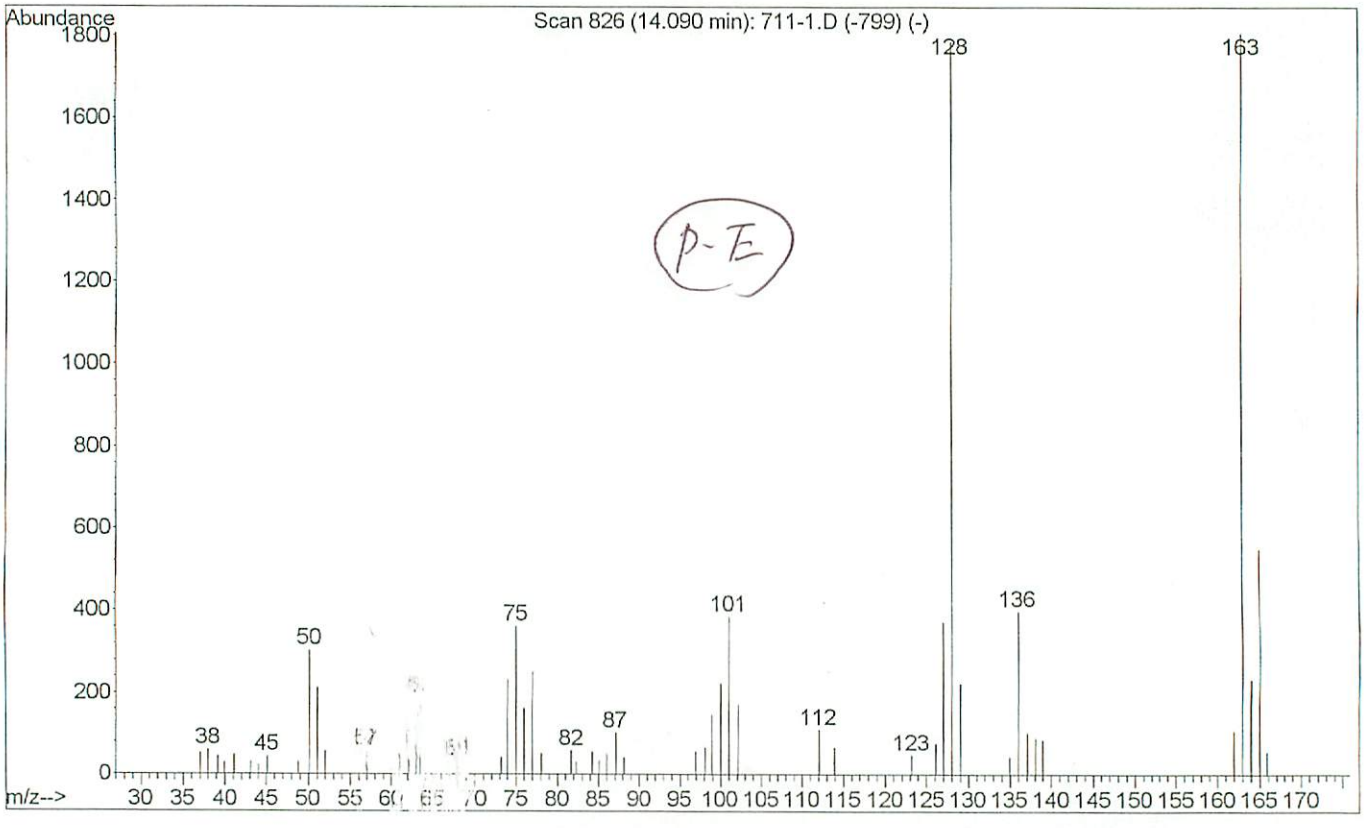


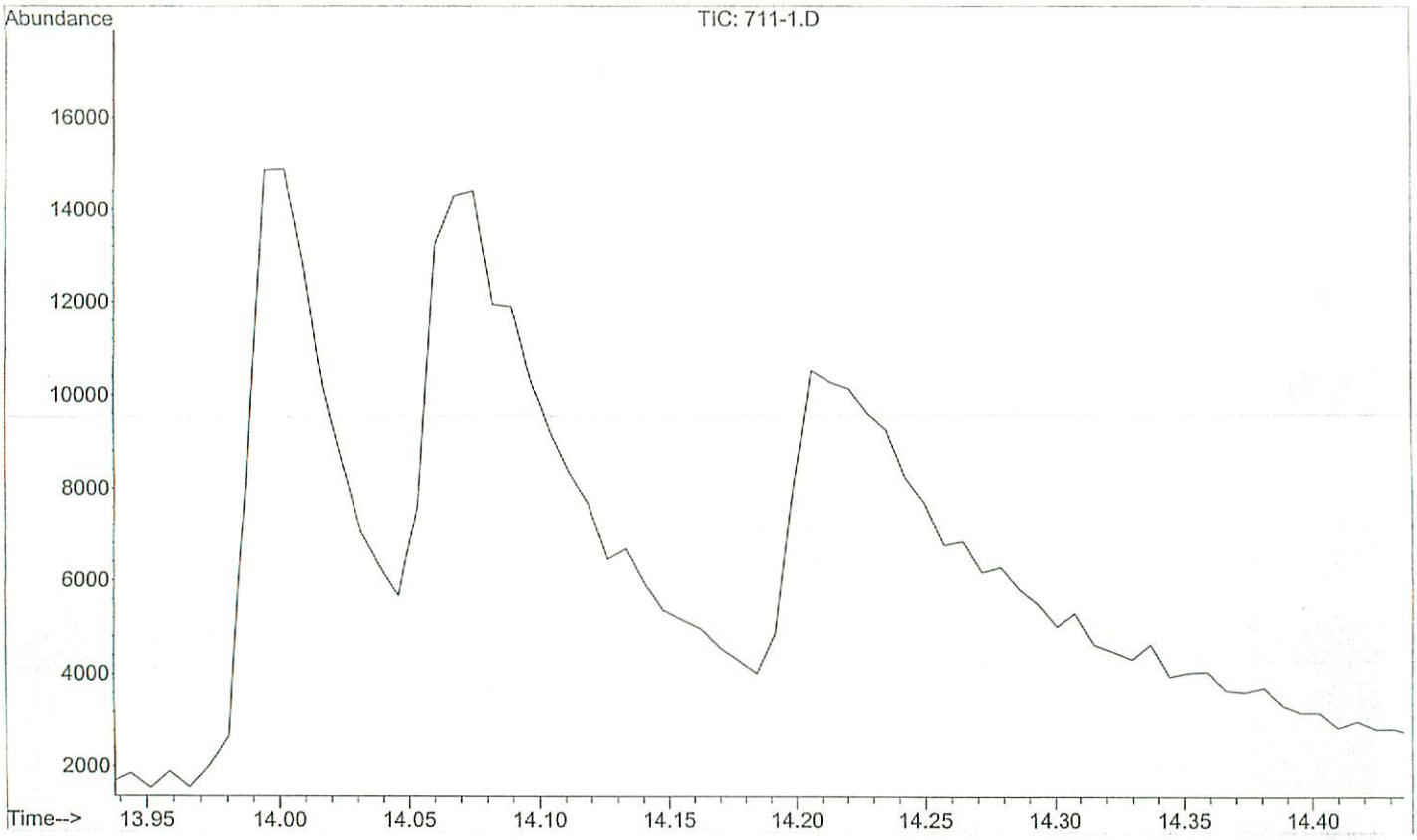


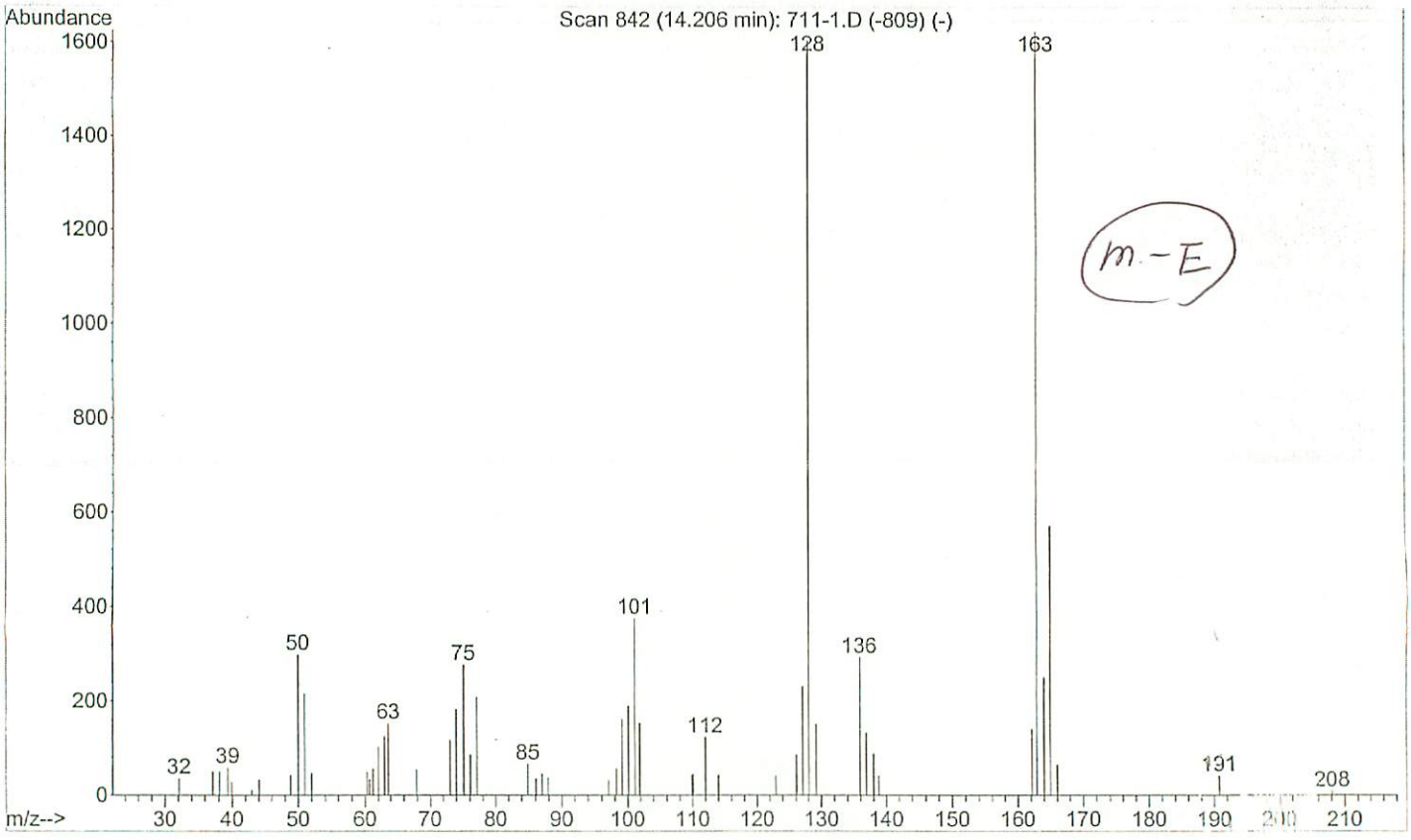
This journal is (c) The Royal Society of Chemistry 2010

```
File        : D:\FINE DATA\OKABE\711-1.D
Operator    :
Acquired    :  9 Sep 2008  21:29     using AcqMethod OKABE
Instrument  :    Instrumen
Sample Name: 711-1
Misc Info   :
Vial Number: 11
```





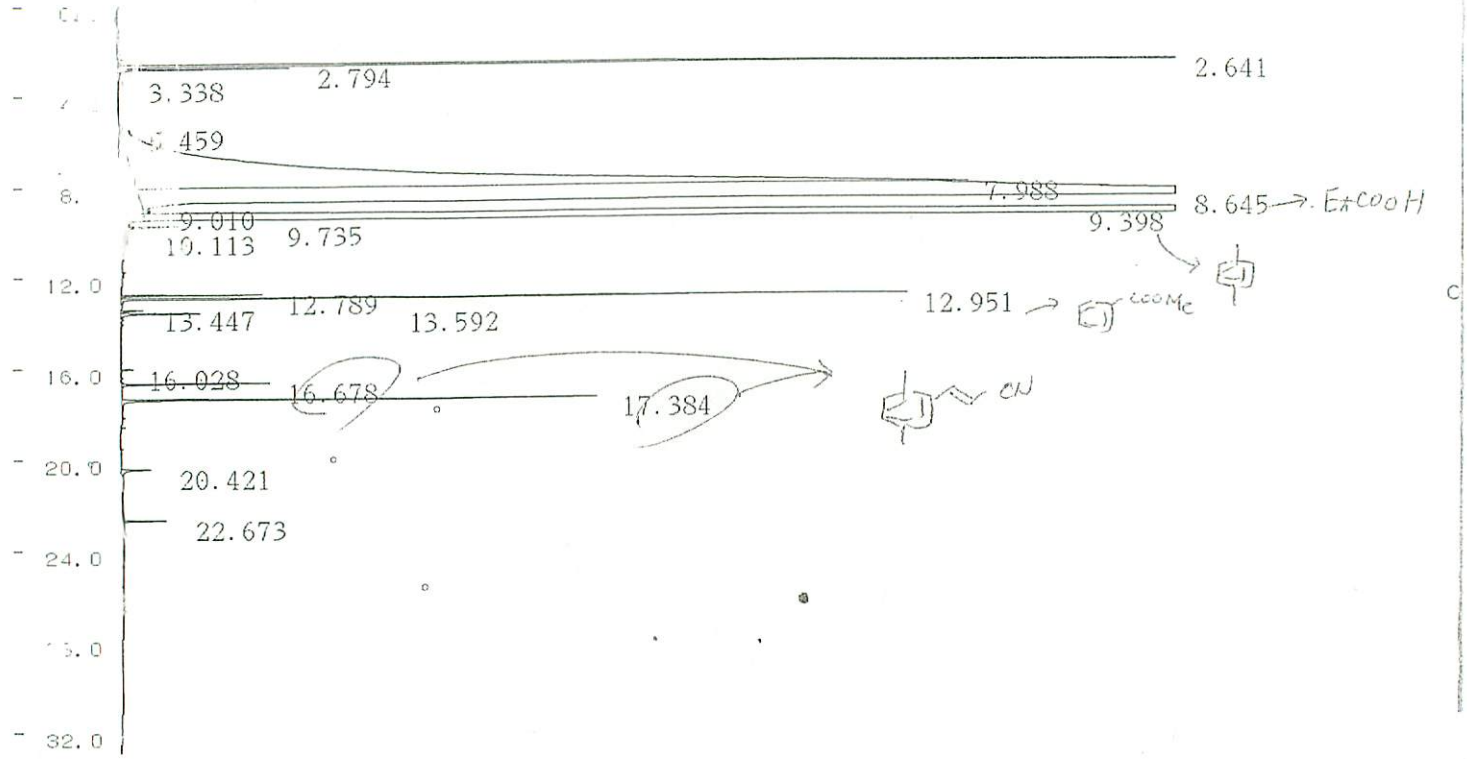

Abundance
TIC: 711-1.D
16000
14000
12000
10000
8000
6000
4000
2000
Time-->
13.95
14.00
14.05
14.10
14.15
14.20
14.25
14.30
14.35
14.40


Abundance
Scan 842 (14.206 min): 711-1.D (-809) (-)
1600
1400
1200
1000
800
600
400
200
0
m/z-->
128
163
101
50
75
136
63
112
85
32
39
191
208
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
m-E

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

Table 2 entry 7

CHROMATOPAC C-R7A CH=1 REPORT No.=4 ｸﾛﾏﾄ=2:1140OK.C00 /10/19 14:58:10



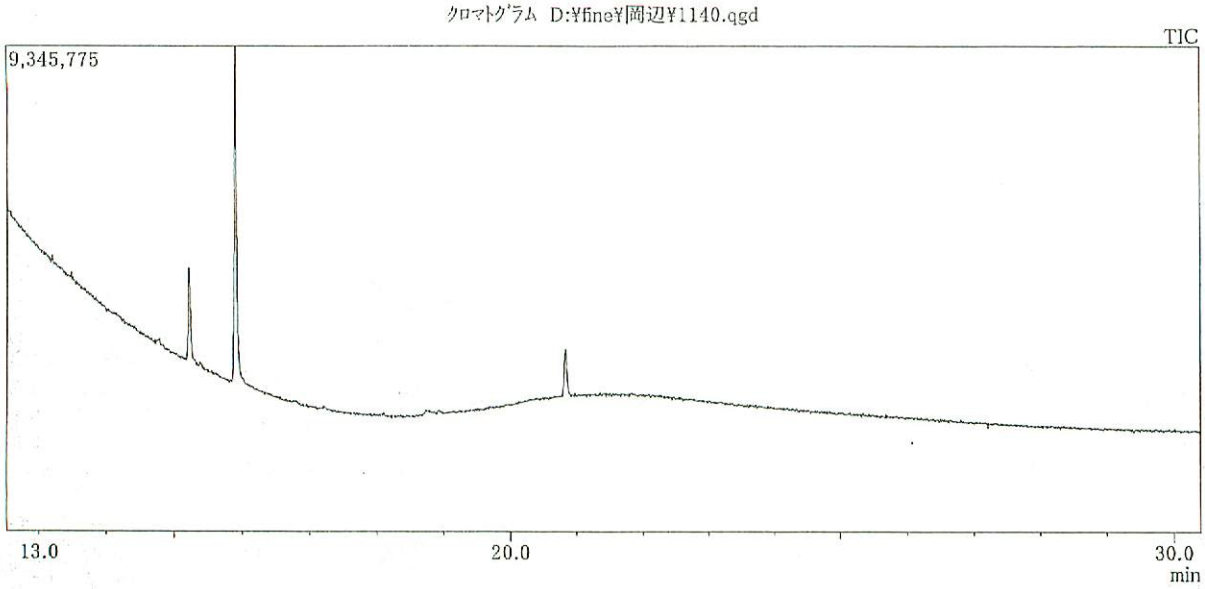
** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	3	2.641	2937864	1345254	SV		17.6082	
	4	2.794	20272	9804	T		0.1215	
	5	3.338	3626	260	T		0.0217	
	7	5.459	5907	582	T		0.0354	
	8	7.988	1776419	50122	TV		10.647	
	9	8.645	2714278	116638	TV		16.2681	
	10	9.01	2049	429	T		0.0123	
	11	9.398	8970020	1029887	SV		53.7621	
	12	9.735	6595	2980	T		0.0395	
	13	10.113	1105	526	T		0.0066	
	19	12.789	17311	8416			0.1038	
	20	12.951	105376	47437	SV		0.6316	
	22	13.447	3548	1295			0.0213	
	23	13.592	13439	4774	V		0.0805	
	28	16.028	1679	743	V		0.0101	
	32	16.678	19685	8883			0.118	
	33	17.384	70994	28566	S		0.4255	
	38	20.421	7345	1771			0.044	
	40	22.673	7157	2606			0.0429	
		TOTAL	16681[illegible]2660971				100	

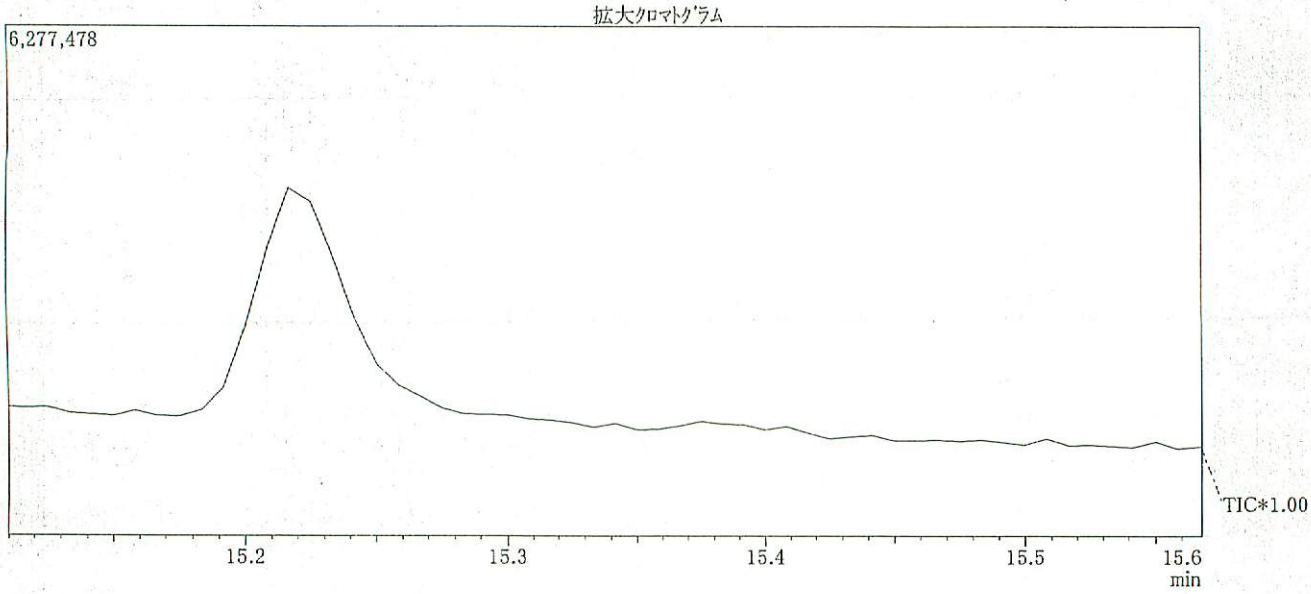
2009/10/20 10:26:20

D:¥fine¥岡辺¥1140.qgd

クロマトグラム D:¥fine¥岡辺¥1140.qgd

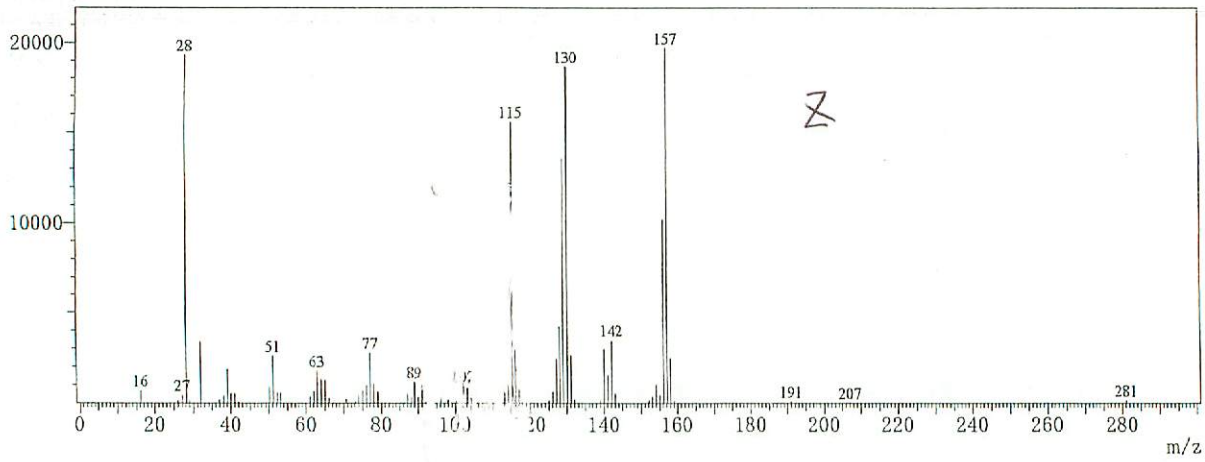


拡大クロマトグラム



スペクトル

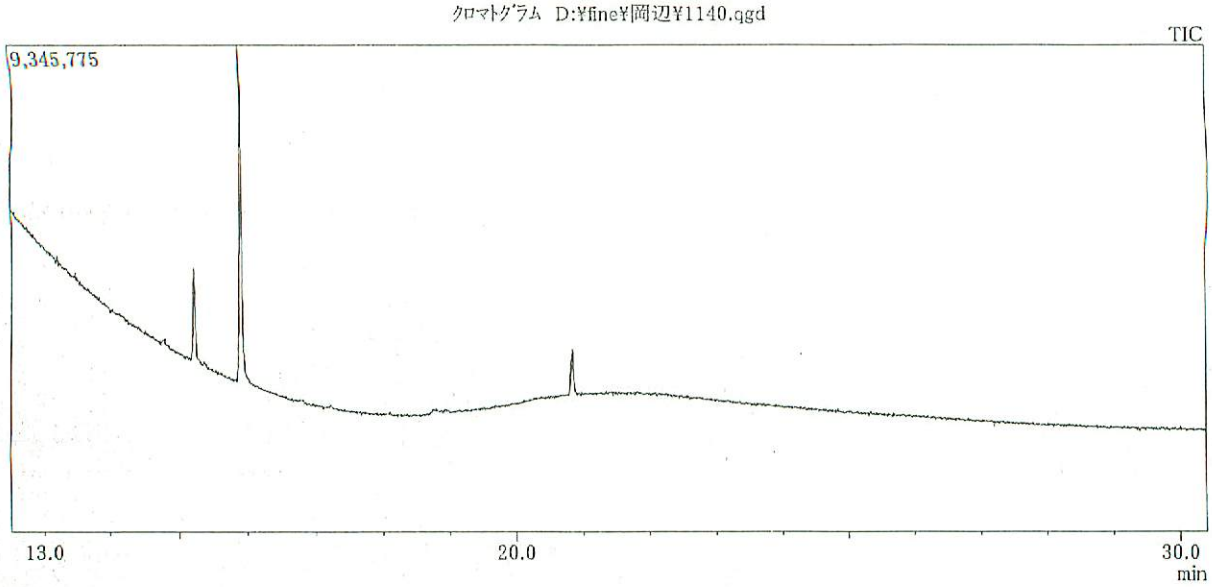
#:1 保持時間:15.217(スキャン#:327)
ピーク数:77 ベースピーク:157.10(19709)
スペクトル:平均 15.175-15.283(322-335)
バックグラウンド:平均 15.225-15.300(328-337)



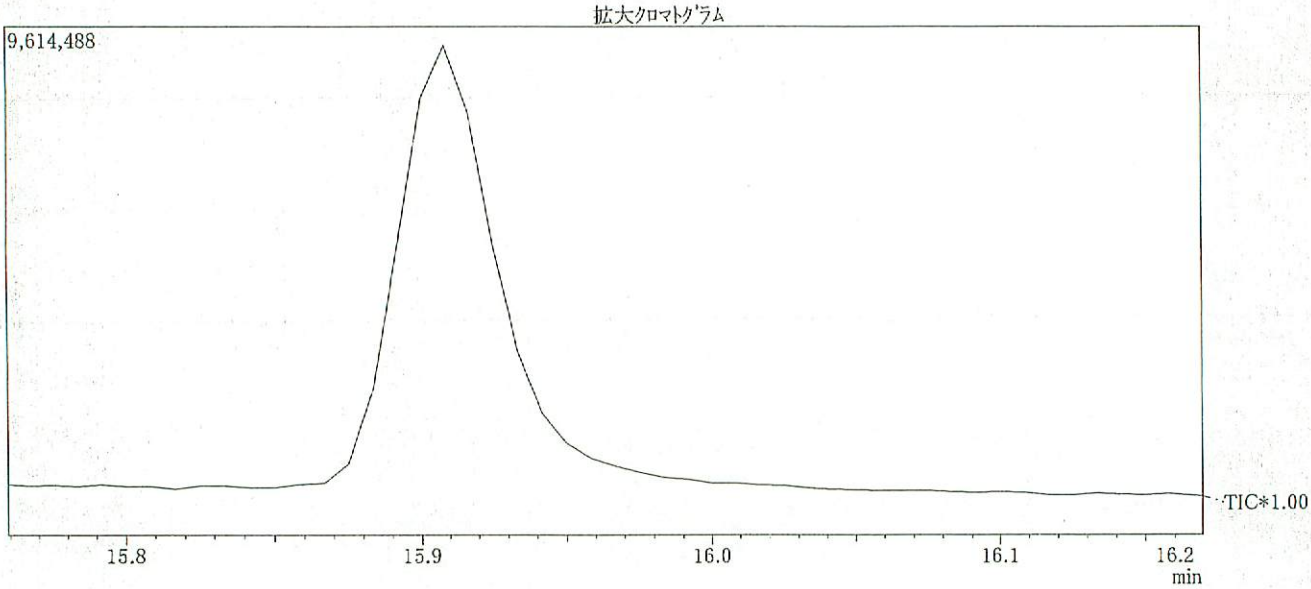
2009/10/20 10:26:38

D:¥fine¥岡辺¥1140.qgd

クロマトグラム D:¥fine¥岡辺¥1140.qgd

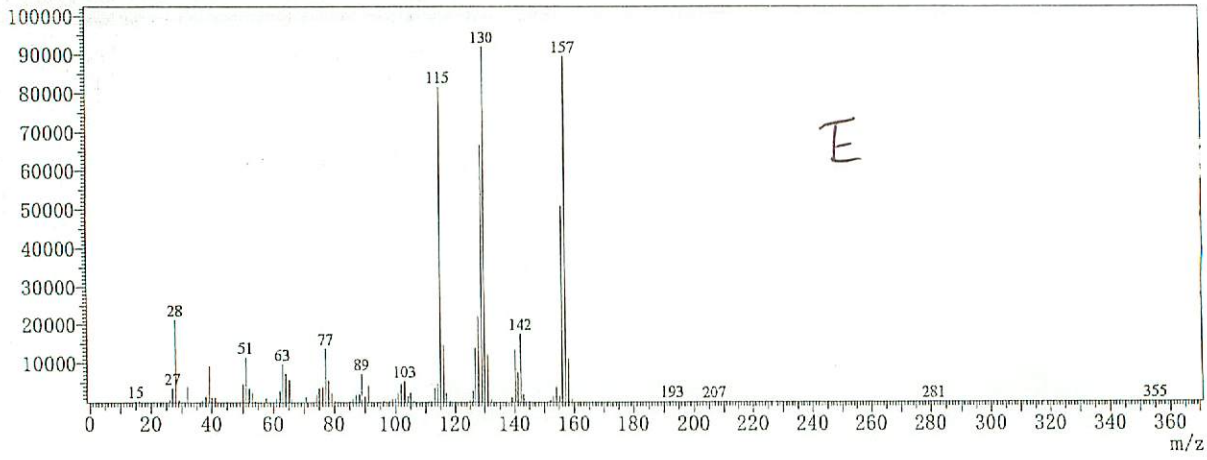


拡大クロマトグラム



スペクトル

#:1 保持時間:15.908(スキャン#:410)
ピーク数:98 ベースピーク:130.10(92083)
スペクトル:平均 15.858-15.975(404-418)
バックグラウンド:平均 15.917-15.992(411-420)



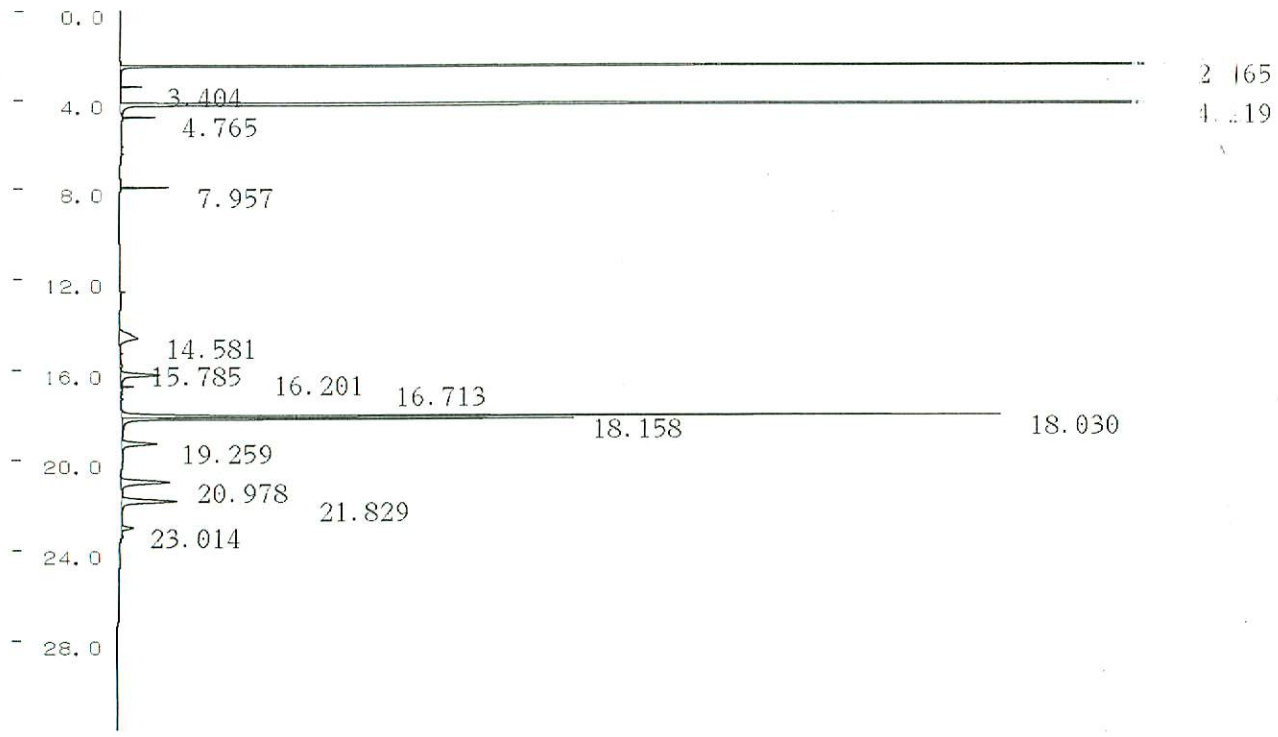
E

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

Table 3 entry 1

極性 GC 純品

CHROMATOPAC C-R7A CH=2 REPORT No.=5 クロマト=2:BE-CRT.C04 10/03/16 17:46:38



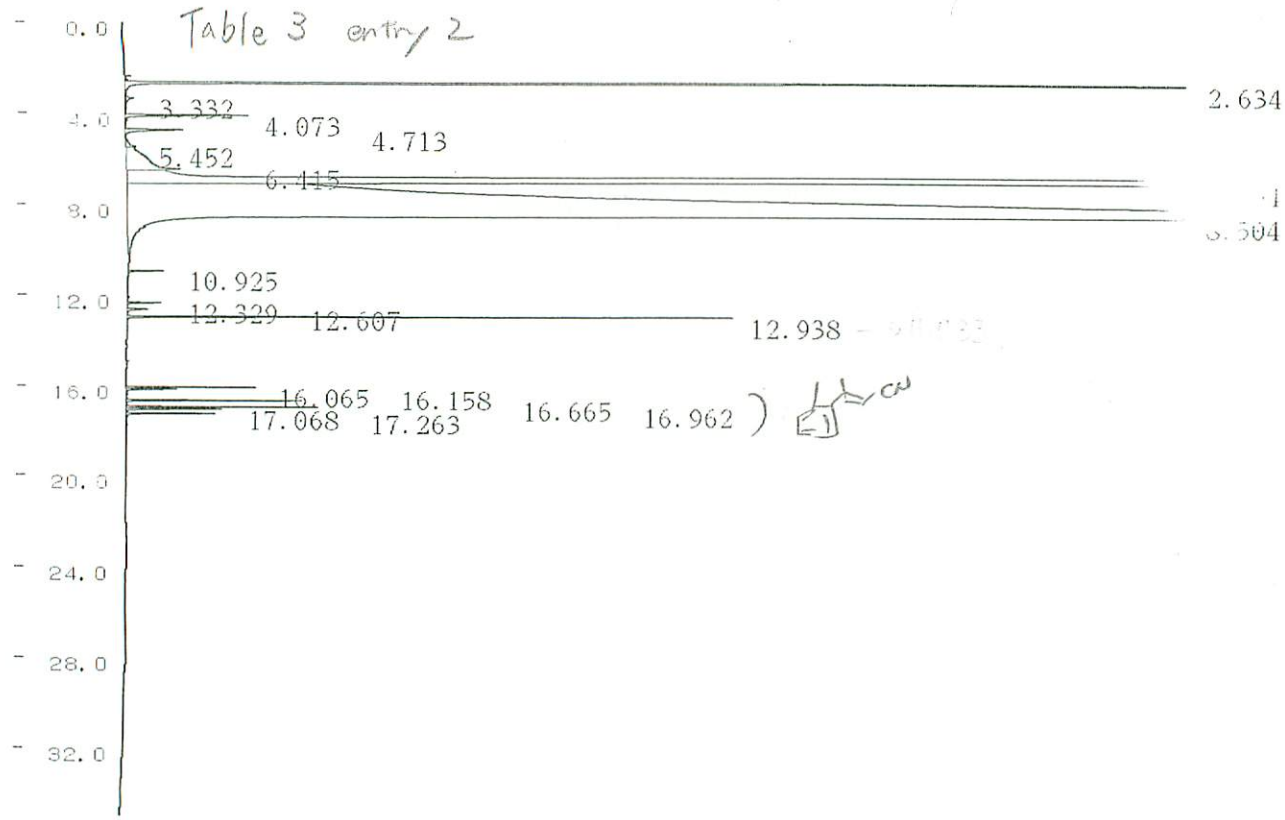
** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
2	1	2.465	8688176	4249478			81.2291	
	2	3.404	2401	1300	L		0.0224	
	4	4.219	1595989	484574	L		14.9215	
	5	4.765	4242	1980	LV		0.0397	
	9	7.957	6158	2868			0.0576	
	13	14.581	20601	1090			0.1926	
	15	15.785	1303	101			0.0122	
	16	16.201	22831	2331	V		0.2135	
	17	16.713	1840	691	V		0.0172	
	20	18.03	174912	53070			1.6353	
	21	18.158	83729	27059	V		0.7828	E
	22	19.259	19583	2046			0.1831	Z
	23	20.978	32428	2885			0.3032	
	24	21.829	35801	3309			0.3347	
	25	23.014	5910	693			0.0553	
		TOTAL	10695896	4833472			100	

68

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

CHROMATOPAC C-R7A CH=1 REPORT No.=8 ﾁｬﾈﾙ=2: 11219R.001 09/10/05 10:24:34



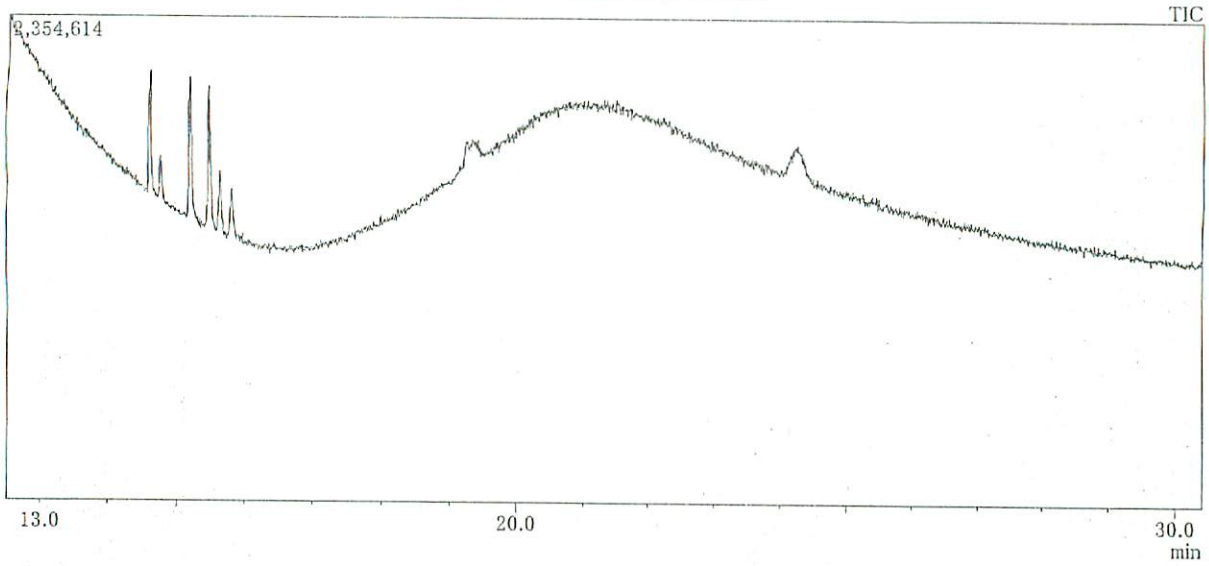
** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	3	2.634	2761001	1383354	V		18.2187	
	4	3.332	3574	526	L		0.0236	
	7	4.073	24950	7414	L		0.1646	
	9	4.713	16840	3461	LV		0.1111	
	10	5.452	1470	571	V		0.0097	
	11	6.415	79663	3220	V		0.5257	
	12	6.994	7772426	983744	V		51.2869	
	13	8.504	4302476	137159	SV		28.3902	
	18	10.925	5357	2170			0.0353	
	20	12.329	5167	2042	V		0.0341	
	21	12.607	4890	1310			0.0323	
	22	12.938	76368	36534	V		0.5039	
	6	16.065	17419	7849			0.1149	
	7	16.158	7882	3092	V		0.052	
		16.665	23669	10568	V		0.1562	
	31	16.962	25482	11527	V		0.1681	
	32	17.068	13375	5750	V		0.0883	
	33	17.263	12795	5322	V		0.0844	
		TOTAL	15154793	2605613			100	

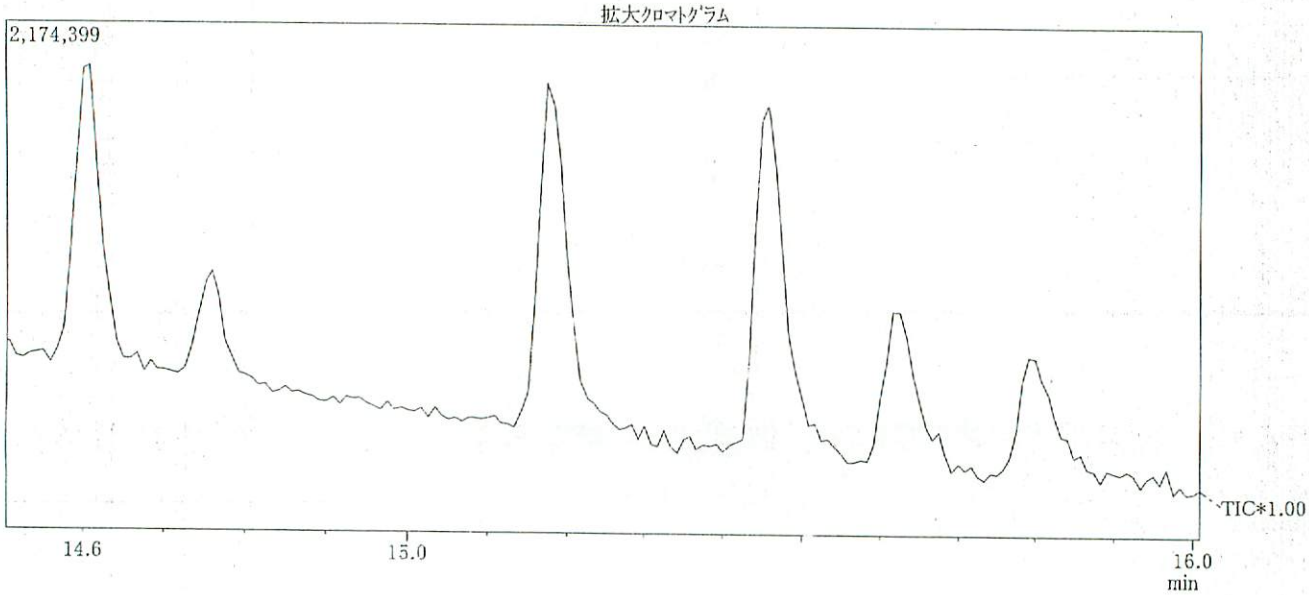
2010/03/16 09:55:10

D:¥fine¥岡辺¥1117.qgd

クロマトグラム D:¥fine¥岡辺¥1117.qgd

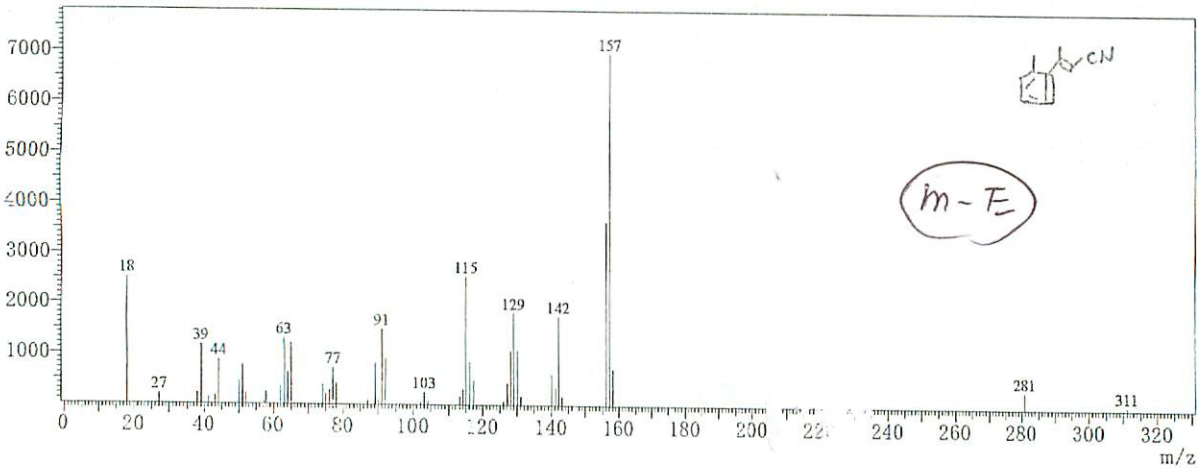


拡大クロマトグラム



スペクトル

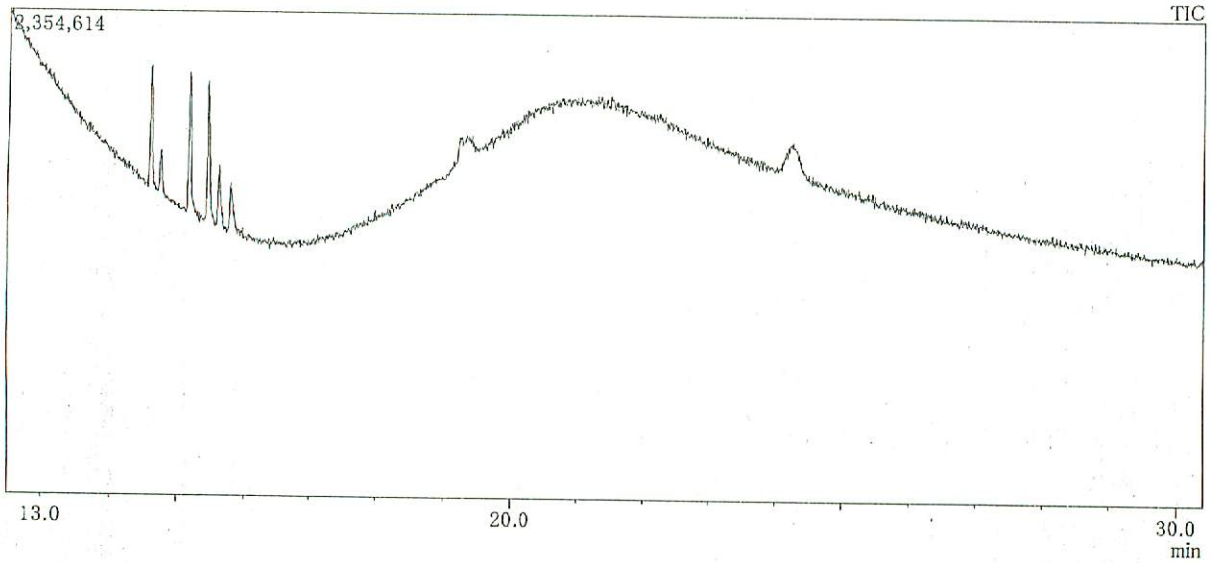
#:1 保持時間:15.792(スキャン#:396)
ピーク数:52 ベースピーク:157.10(6979)
スペクトル:平均 15.750-15.883(391-407)
バックグラウンド:平均 15.742-15.783(390-395)



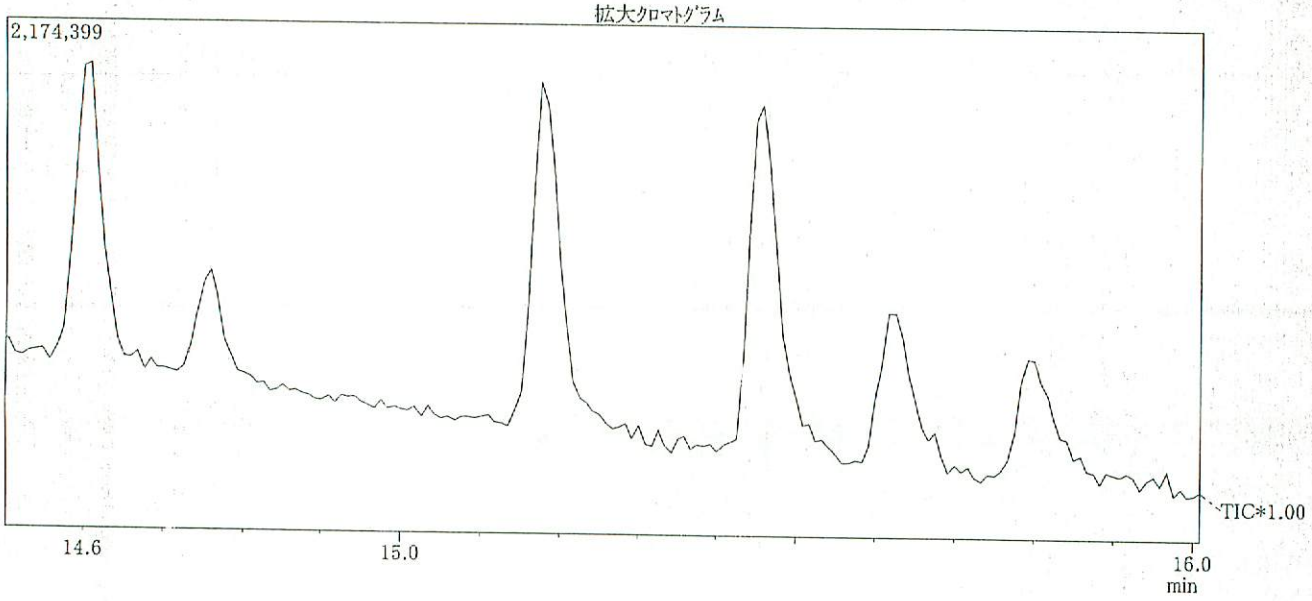
2010/03/16 09:54:54

D:¥fine¥岡辺¥1117.qgd

クロマトグラム D:¥fine¥岡辺¥1117.qgd

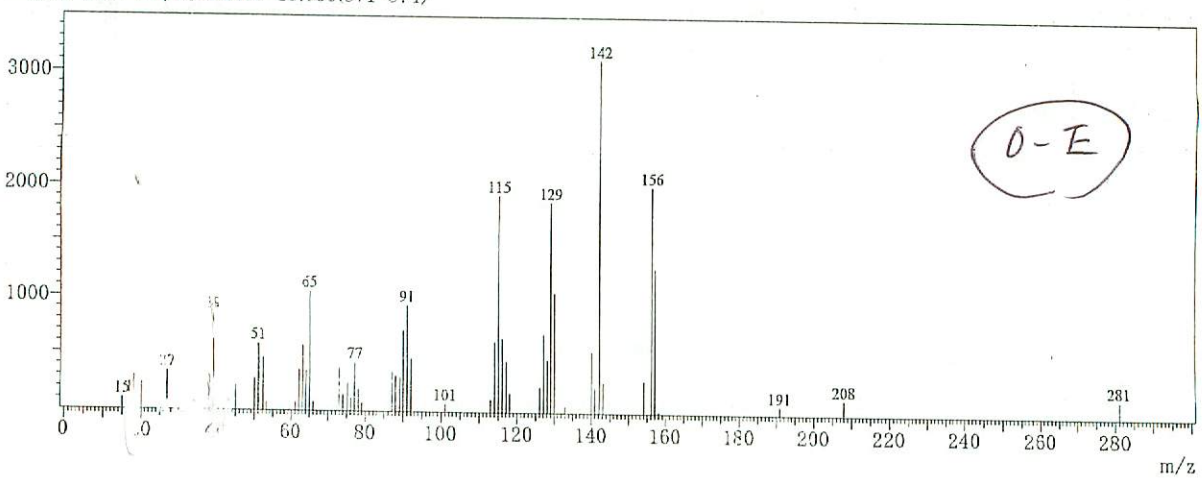


拡大クロマトグラム



スペクトル

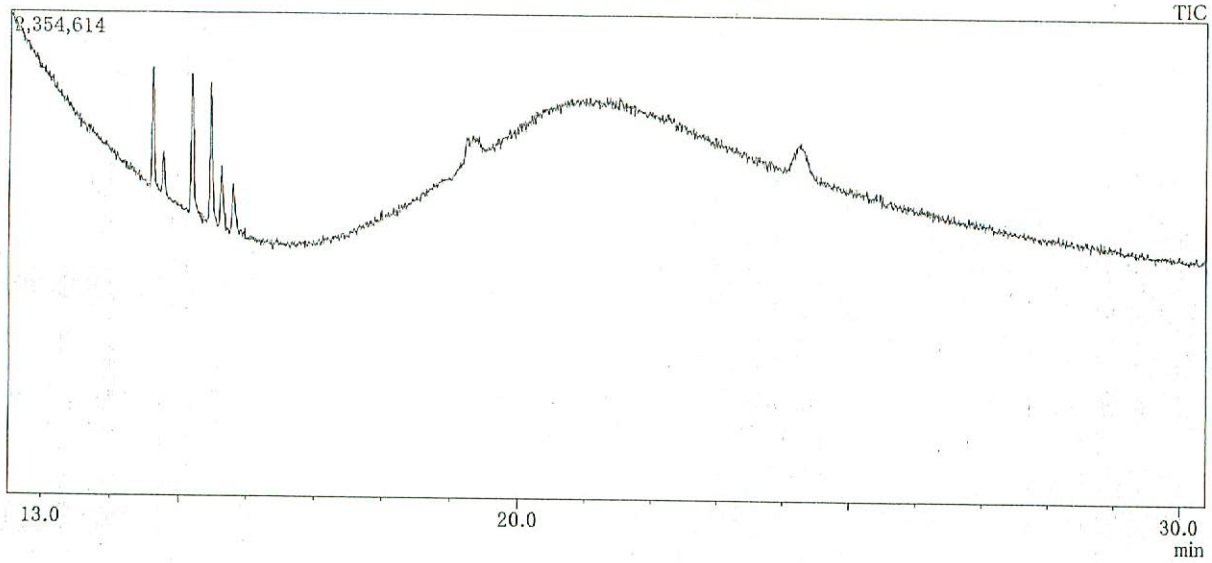
#:1 保持時間:15 625(スキャン#:376)
ピーク数:60 ベースピーク:142.10(3112)
スペクトル:平均 15.575-15.692(370-384)
バックグラウンド:平均 15.583-15.608(371-374)



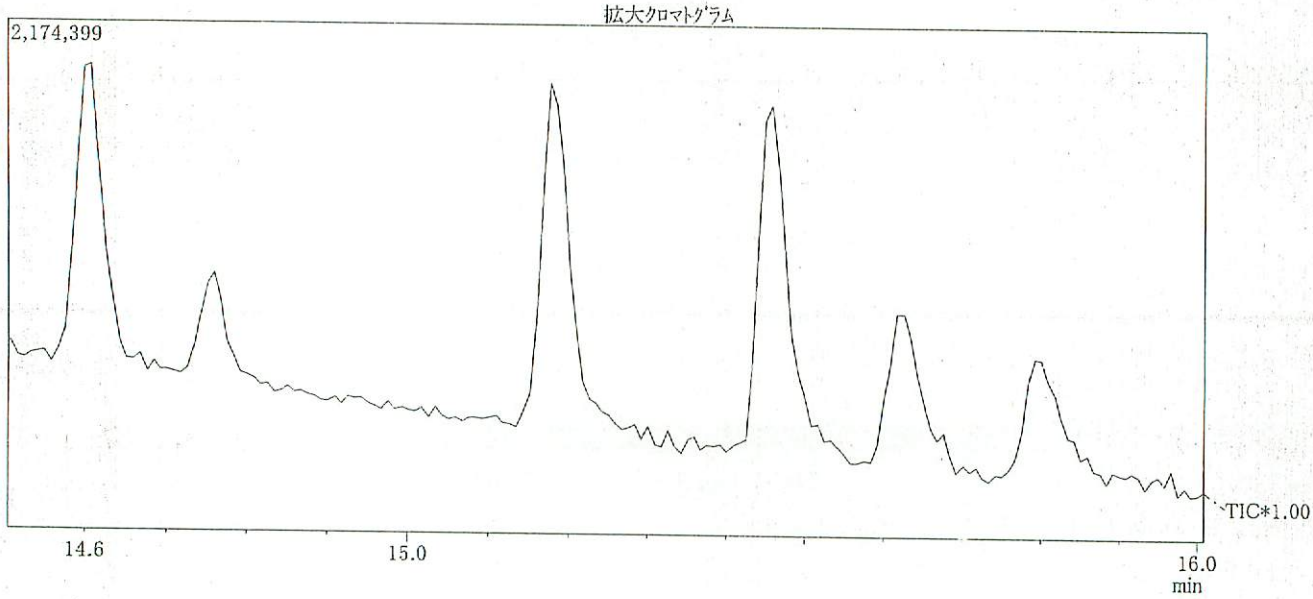
2010/03/16 09:54:36

D:¥fine¥岡辺¥1117.qgd

クロマトグラム D:¥fine¥岡辺¥1117.qgd

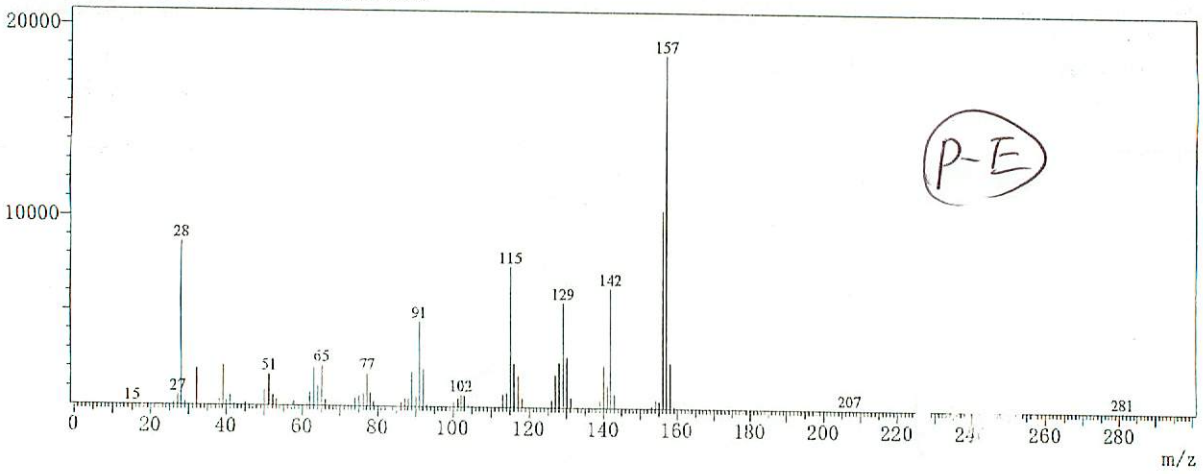


拡大クロマトグラム



スペクトル

#:1 保持時間:15.458(スキャン#:356)
ピーク数:72 ベースピーク:157.05(18520)
スペクトル:平均 15.408-15.553(350-368)
バックグラウンド:平均 15.475-15.567(358-369)

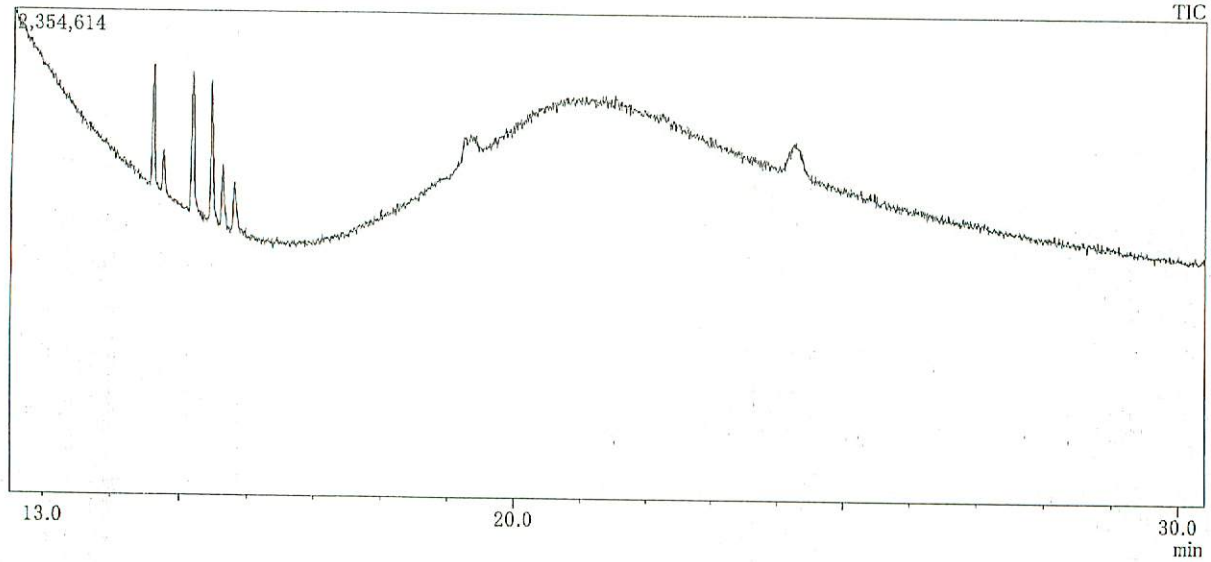


P-E

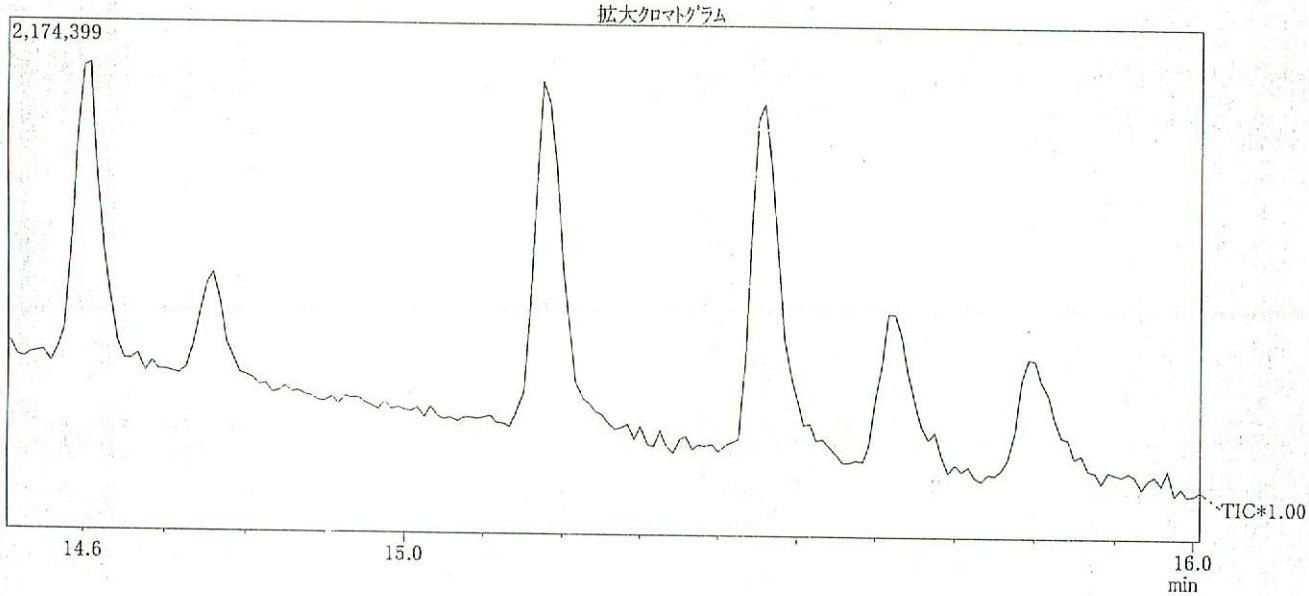
2010/03/16 09:54:13

D:¥fine¥岡辺¥1117.qgd

クロマトグラム D:¥fine¥岡辺¥1117.qgd

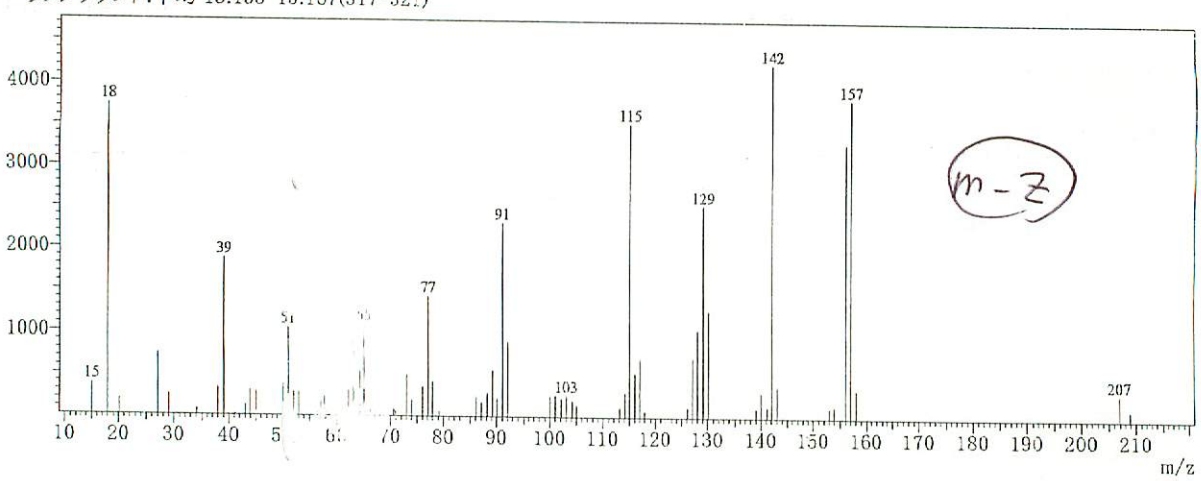


拡大クロマトグラム



スペクトル

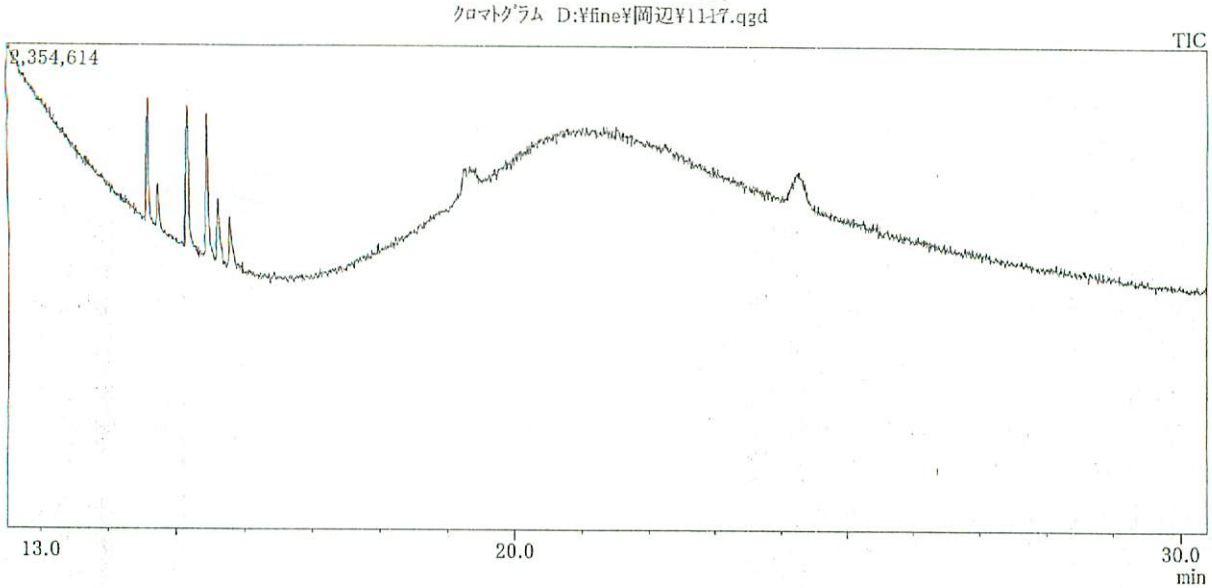
#:1 保持時間:15.175(スキャン#:32)
ピーク数:69 ベースピーク:142.05(4239)
スペクトル:平均 15.125-15.267(316-333)
バックグラウンド:平均 15.133-15.167(317-321)



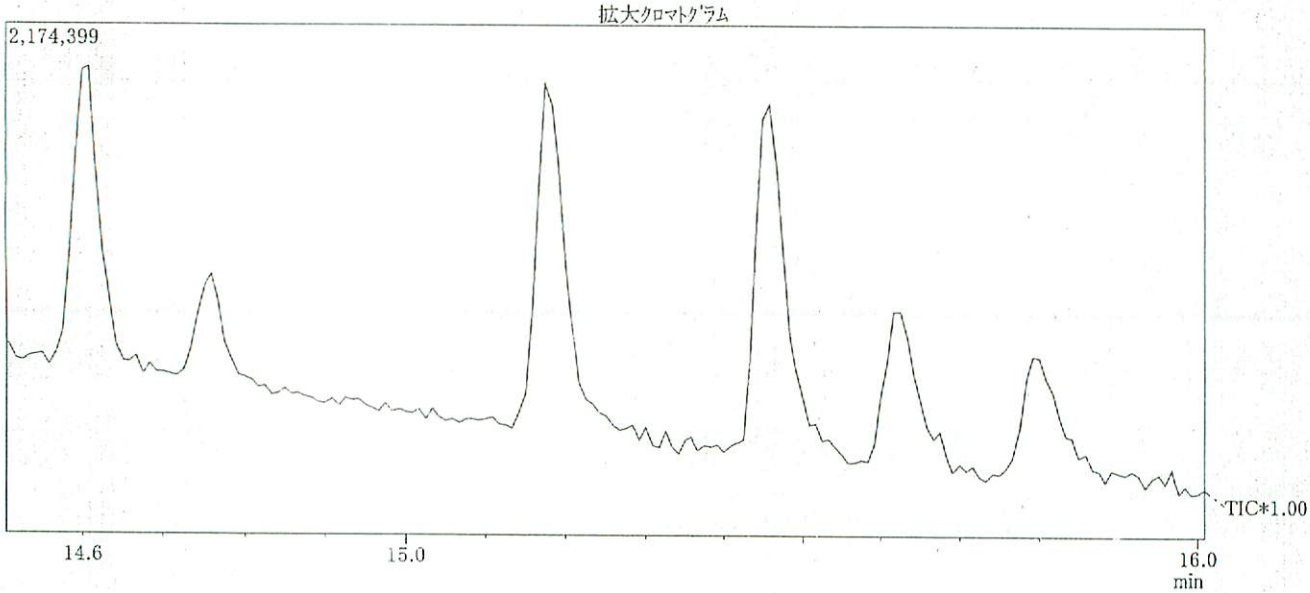
2010/03/16 09:53:59

D:¥fine¥岡辺¥1117.qgd

クロマトグラム D:¥fine¥岡辺¥1117.qgd

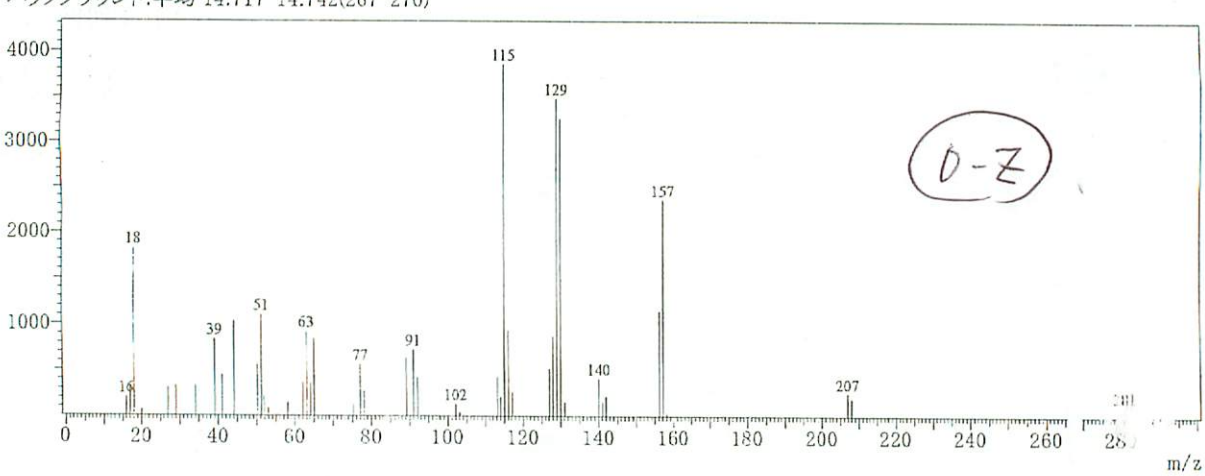


拡大クロマトグラム



スペクトル

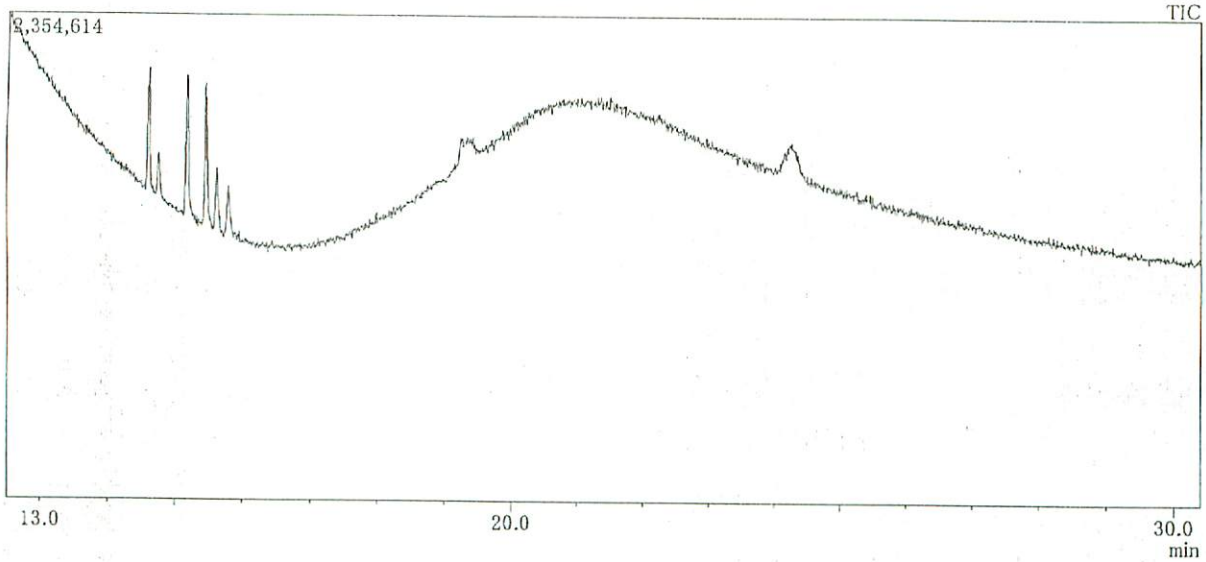
#:1 保持時間:14.758(スキャン#:272)
ピーク数:46 ベースピーク:115.05(3858)
スペクトル:平均 14.717-14.808(267-278)
バックグラウンド:平均 14.717-14.742(267-270)



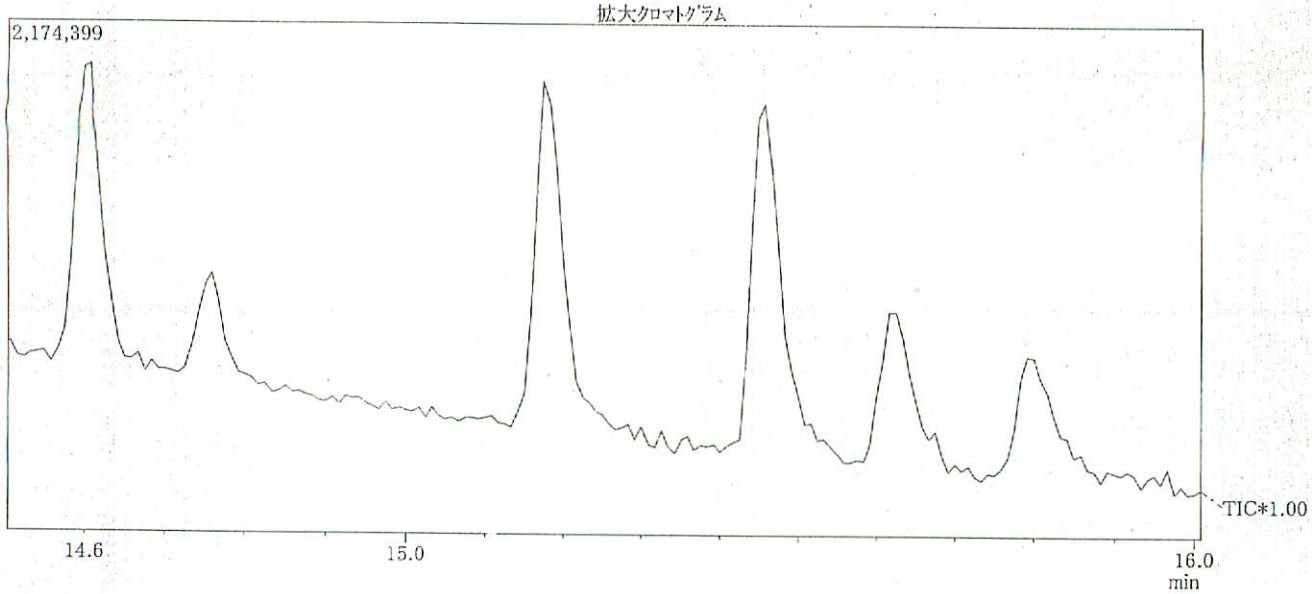
2010/03/16 09:53:43

D:¥fine¥岡辺¥1117.qgd

クロマトグラム D:¥fine¥岡辺¥1117.qgd

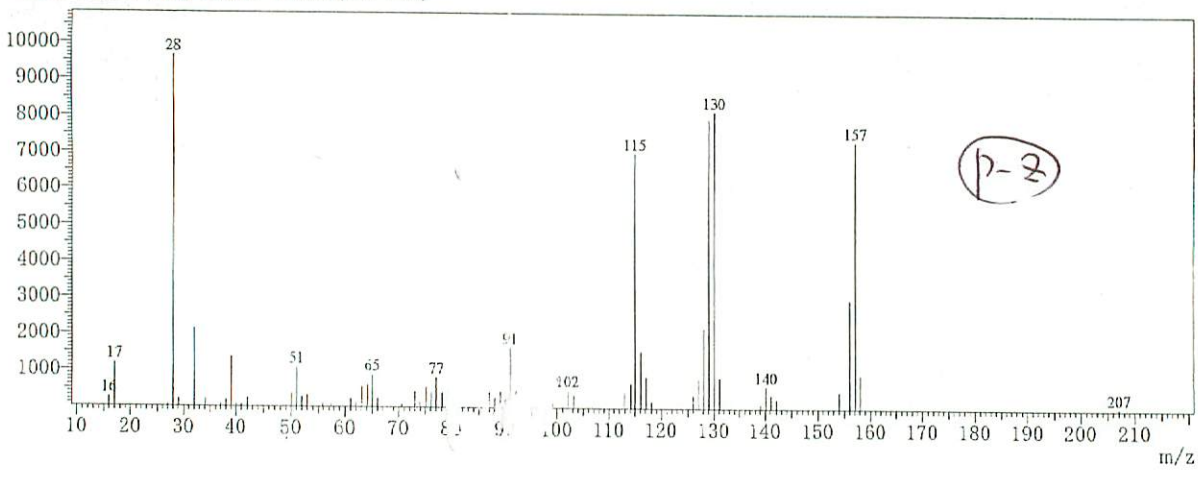


拡大クロマトグラム



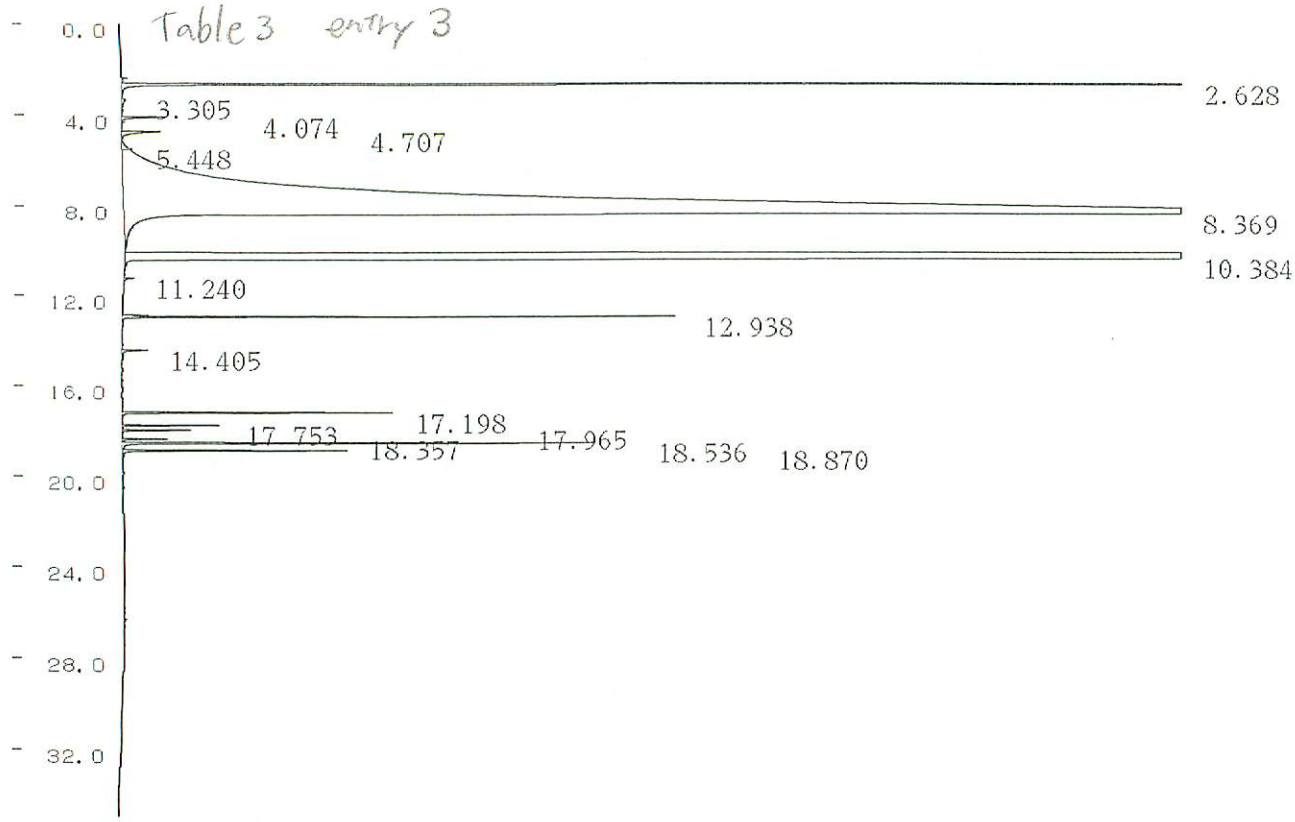
スペクトル

#:1 保持時間:14.608(スキャン#:254)
ピーク数:65 ベースピーク:28.00(9647)
スペクトル:平均 14.558-14.650(248-259)
バックグラウンド:平均 14.617-14.650(255-259)



Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

CHROMATOPAC C-R7A CH=1 REPORT No.=8 ﾌﾟﾛｾｽ=2:1130OK.C00 09/10/06 08:34:28



** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	3	2.628	2206721	1145974	V		15.369	
	4	3.305	2858	234	L		0.0199	
	6	4.074	9817	2614	L		0.0684	
	8	4.707	12598	2346	L		0.0877	
	9	5.448	1173	547	V		0.0082	
	10	8.369	3597610	105265	SV		25.056	
	12	10.384	8274438	852780			57.6284	
	14	11.24	2172	617			0.0151	
	15	12.938	72764	33192			0.5068	
	17	14.405	5135	1527	V		0.0358	
	25	17.198	37071	16055			0.2582	オルト-エ
	26	17.753	12850	5772			0.0895	オルト-エ
	27	17.965	9559	4034	V		0.0666	オルト-エ
	28	18.357	6423	2662			0.0447	オルト-エ
	29	18.536	74289	28212	V		0.5174	オルト-エ
	30	18.87	32801	13336	SV		0.2284	オルト-エ
		TOTAL	14358270	2215164			100	

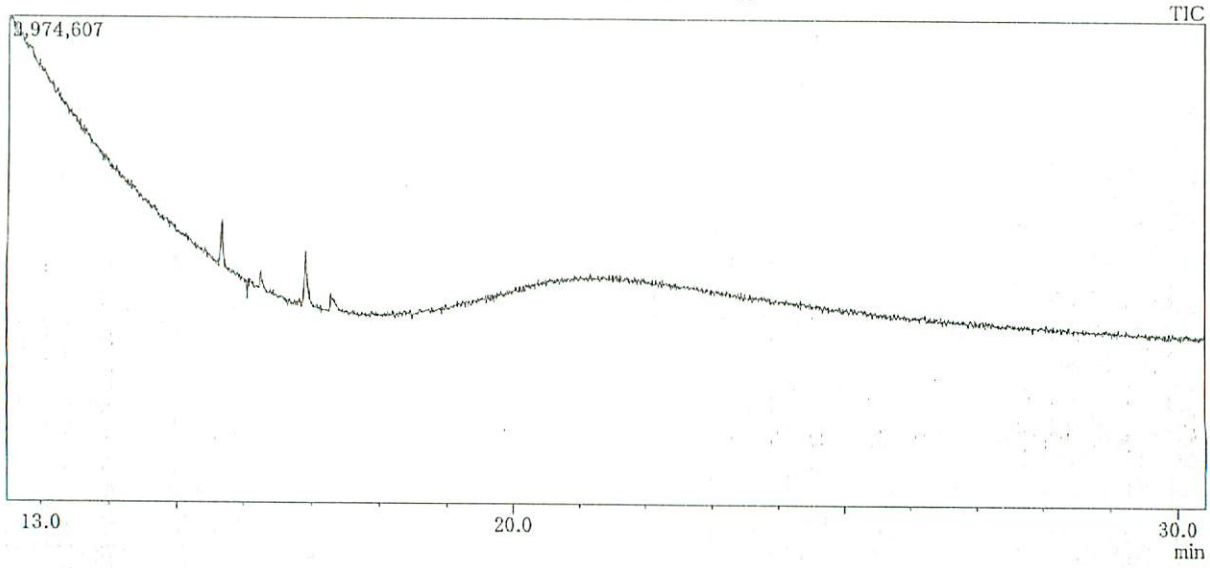
17,2993

1130

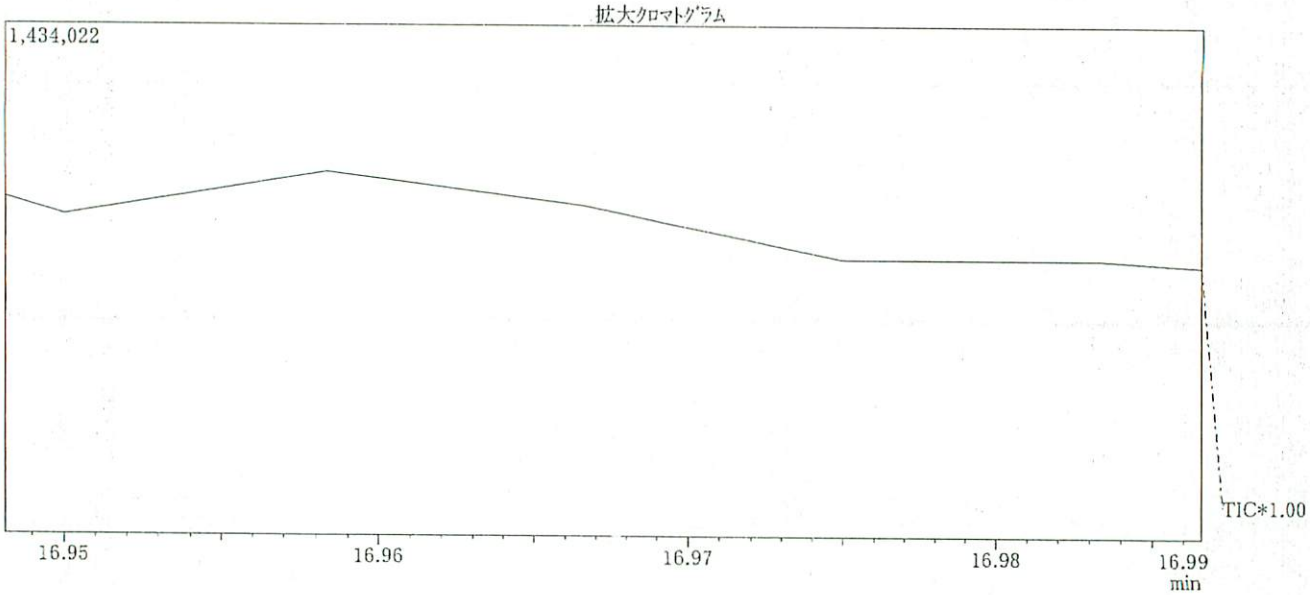
2010/03/16 10:28:57

D:¥fine¥岡辺¥1129.qgd

クロマトグラム D:¥fine¥岡辺¥1129.qgd

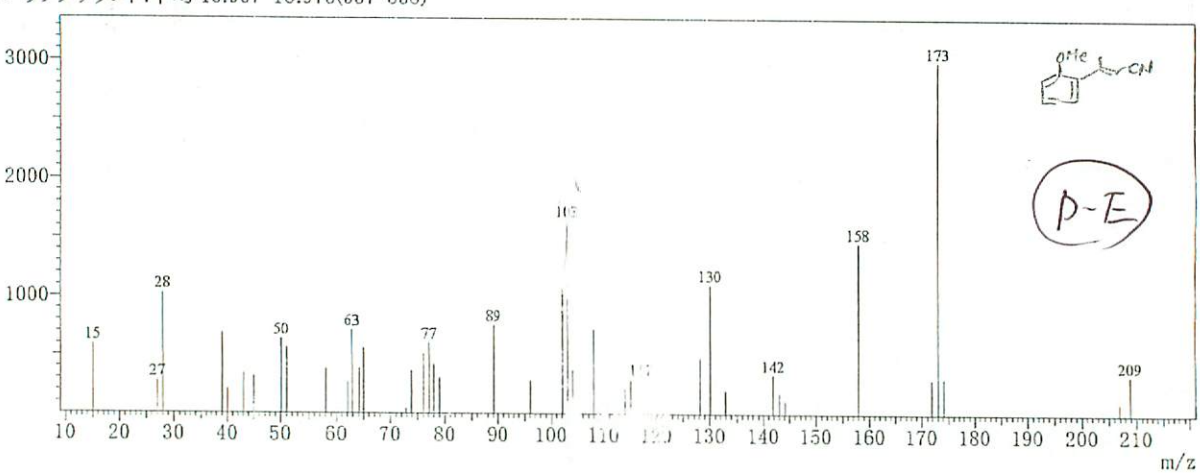


拡大クロマトグラム



スペクトル

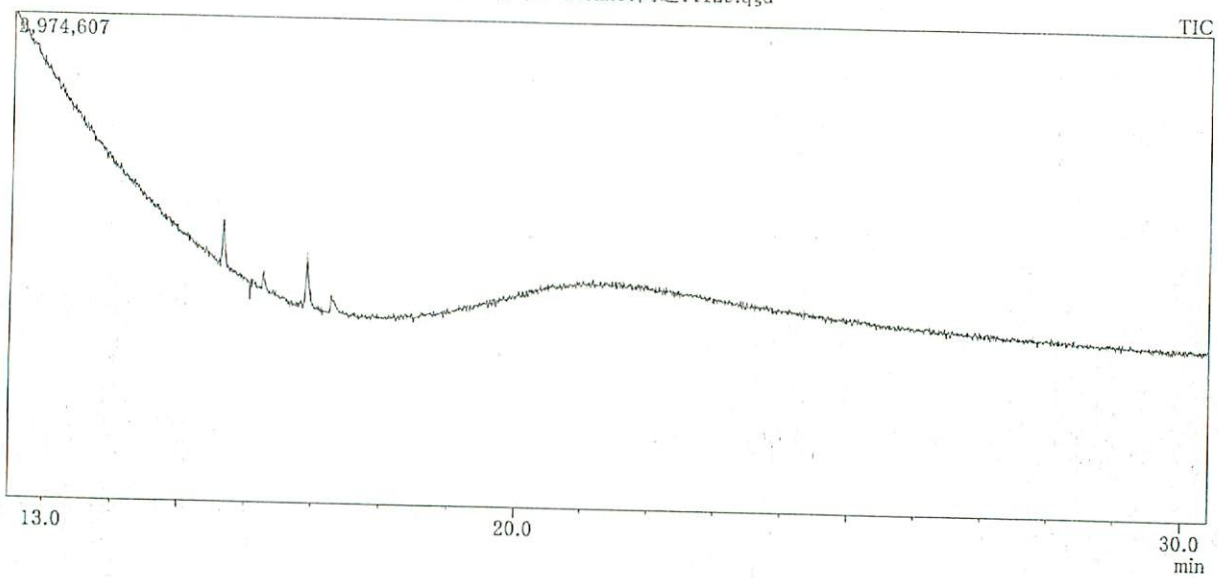
#:1 保持時間:16.958(スキャン#:536)
ピーク数:43 ベースピーク:173.00(2998)
スペクトル:平均 16.950-16.975(535-538)
バックグラウンド:平均 16.967-16.975(537-538)



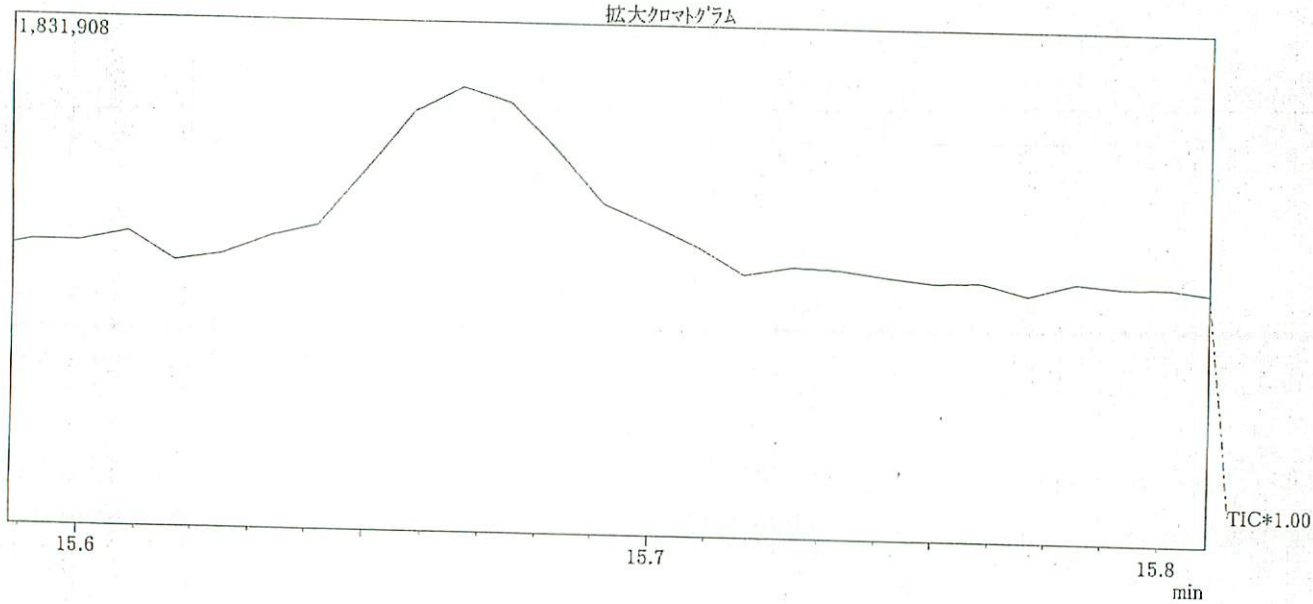
2010/03/16 10:27:29

D:¥fine¥岡辺¥1129.qgd

クロマトグラム D:¥fine¥岡辺¥1129.qgd

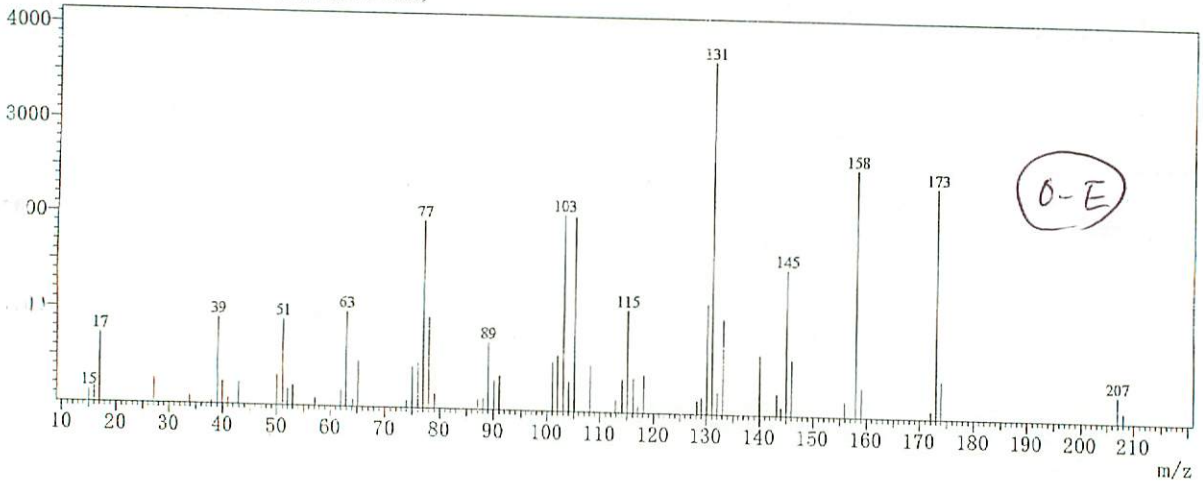


拡大クロマトグラム



スペクトル

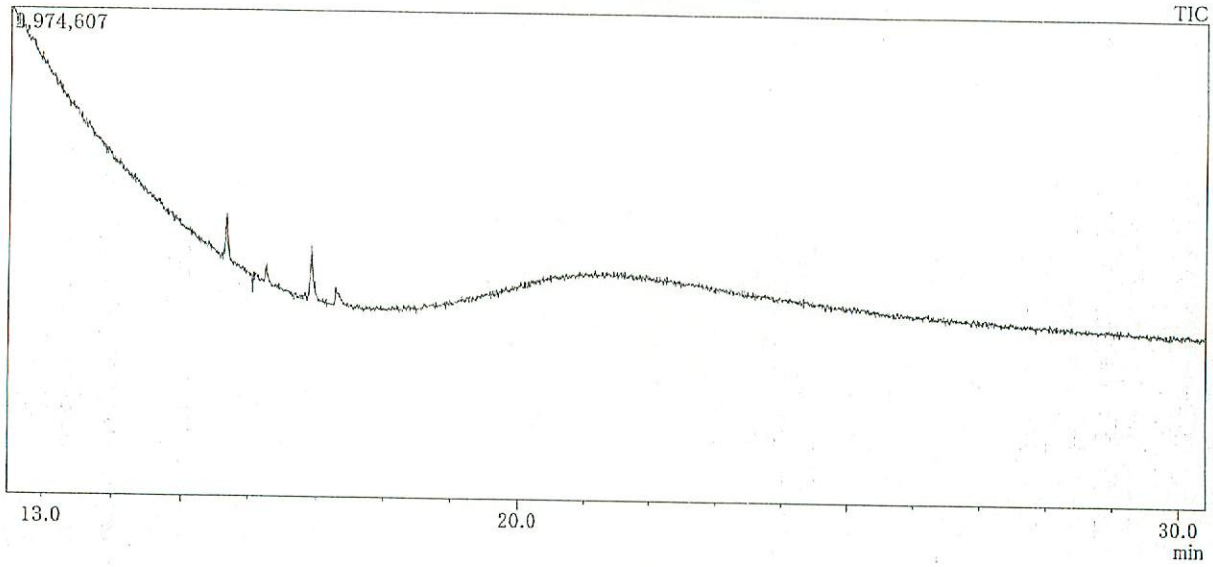
#:1 保持時間:15.667(スキャン#:381)
ピーク数:61 ベースピーク:131.05(3691)
スペクトル:平均 15.617-15.717(375-387)
バックグラウンド:平均 15.617-15.658(375-380)



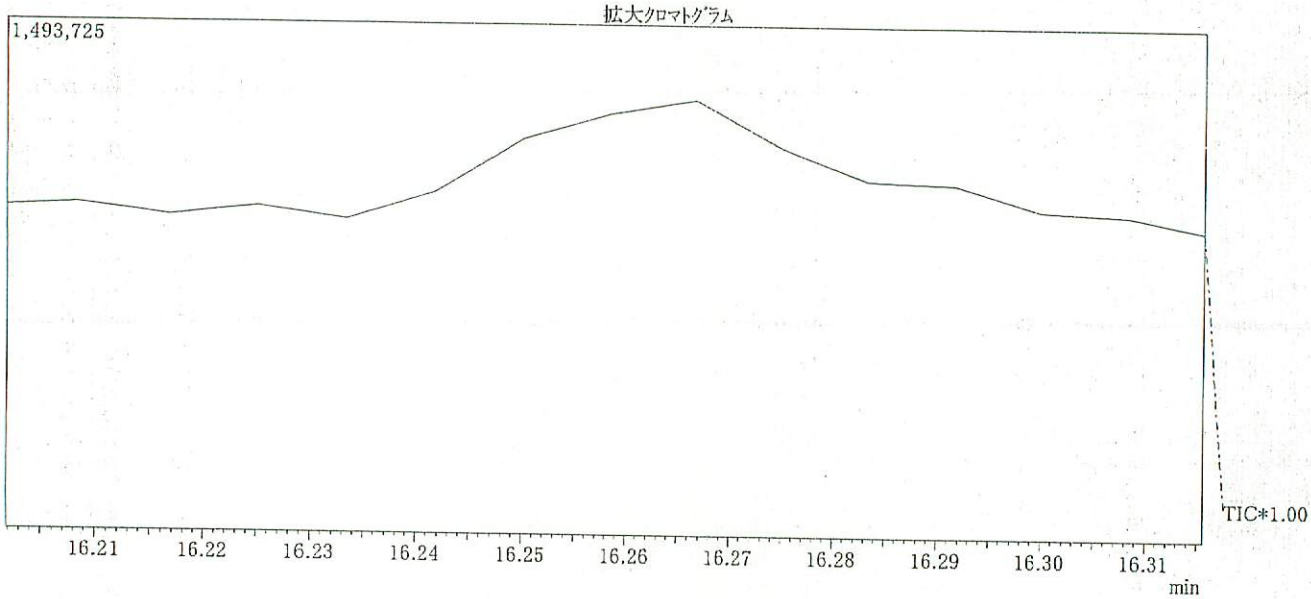
2010/03/16 10:27:59

D:¥fine¥岡辺¥1129.qgd

クロマトグラム D:¥fine¥岡辺¥1129.qgd

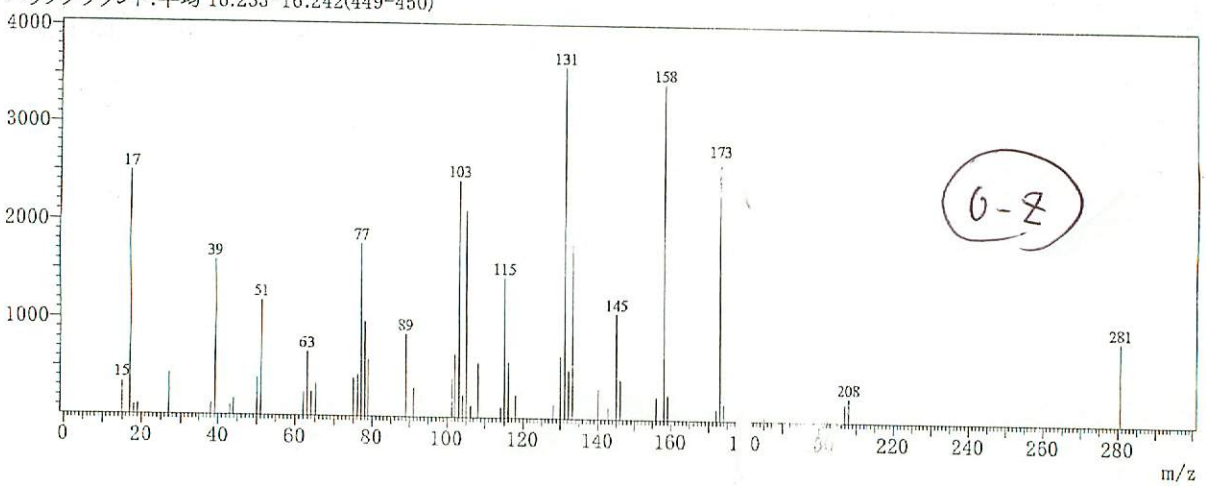


拡大クロマトグラム



スペクトル

#:1 保持時間:16.267(スキャン#:453)
ピーク数:51 ベースピーク:131.05(3600)
スペクトル:平均 16.233-16.308(449-458)
バックグラウンド:平均 16.233-16.242(449-450)

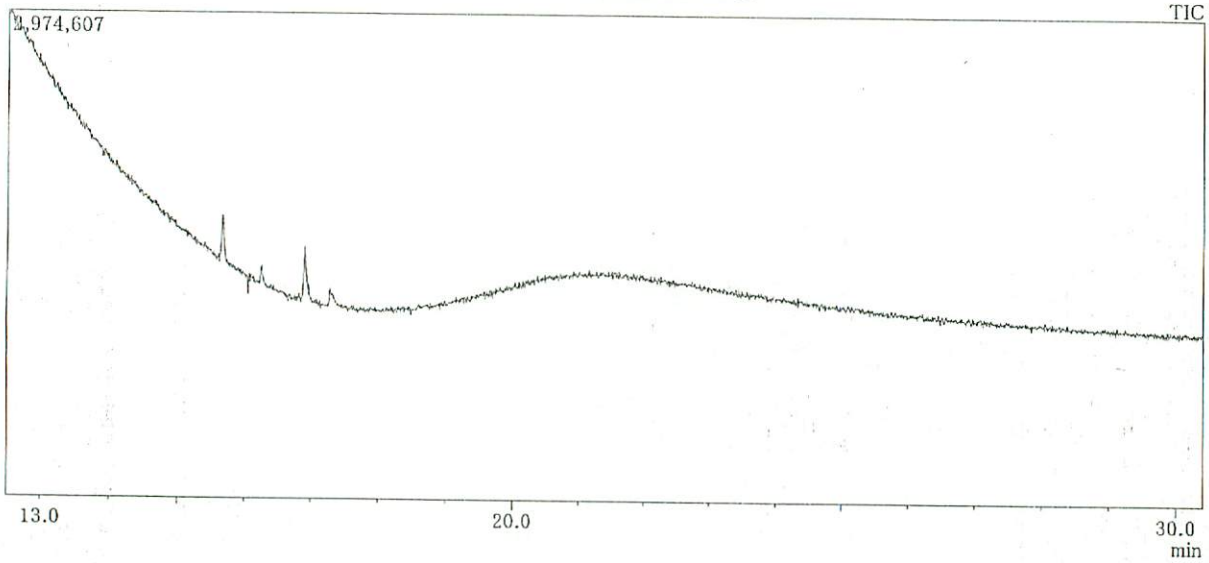


6-8

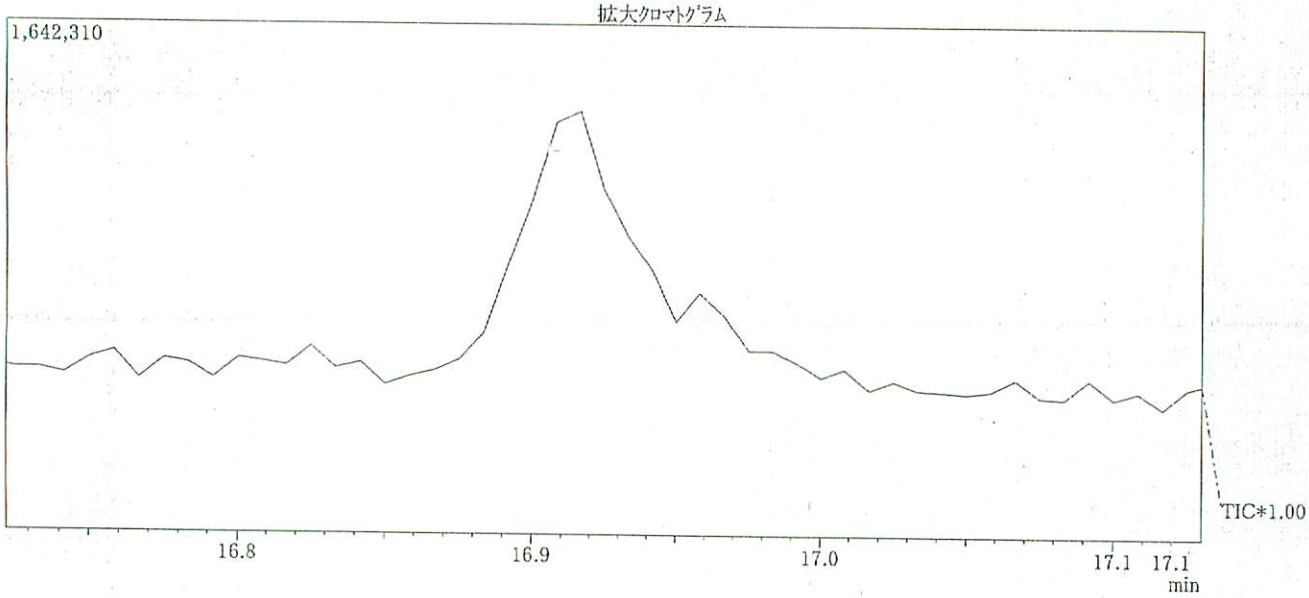
2010/03/16 10:28:32

D:¥fine¥岡辺¥1129.qgd

クロマトグラム D:¥fine¥岡辺¥1129.qgd

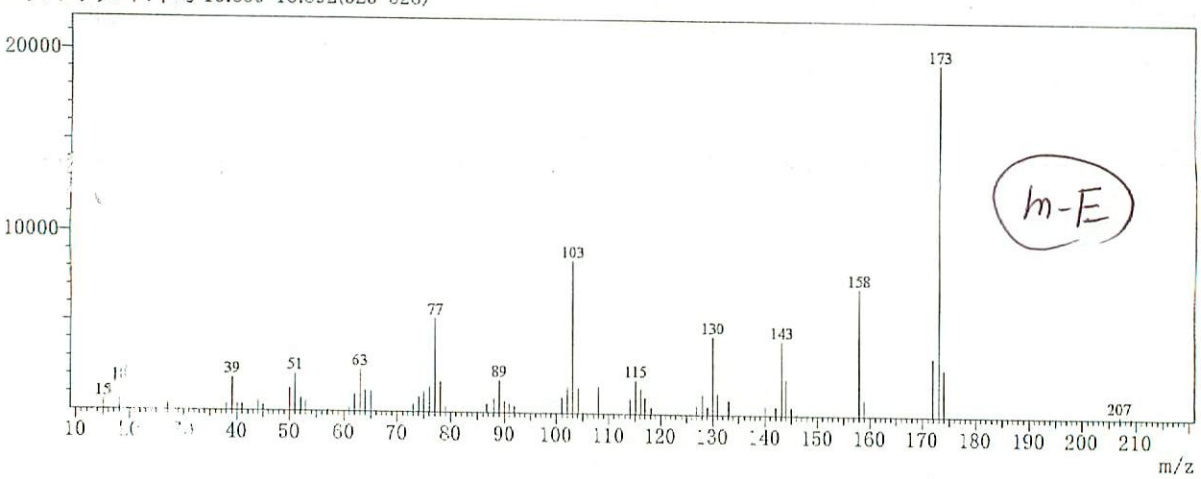


拡大クロマトグラム



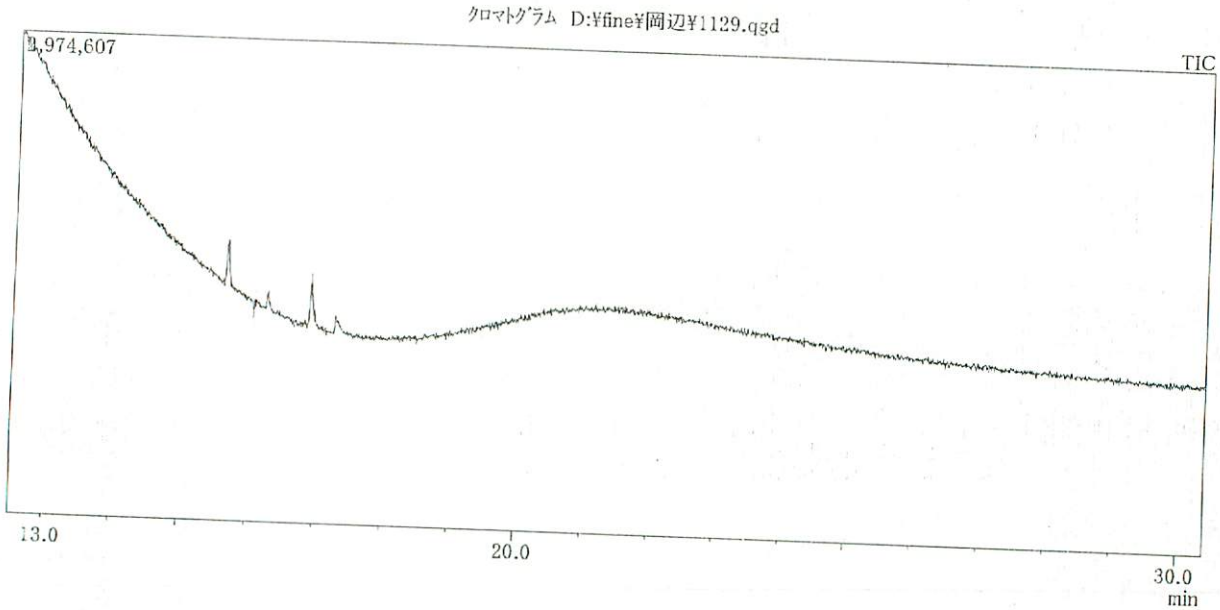
スペクトル

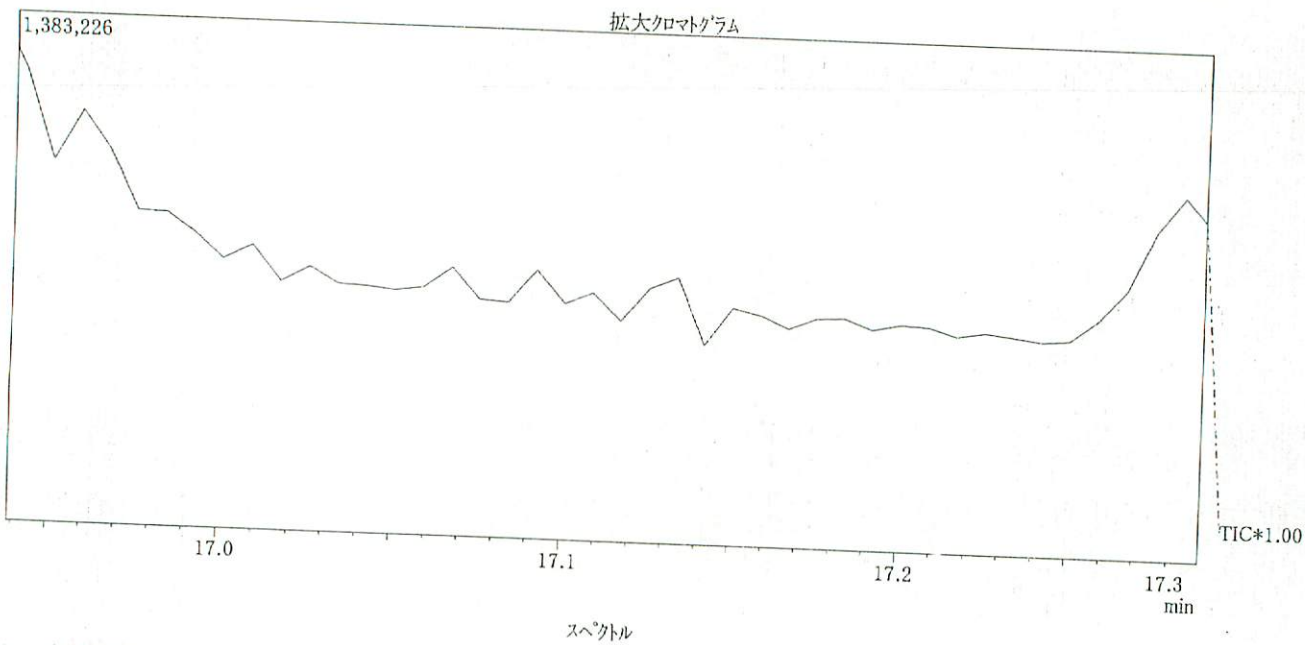
#:1 保持時間:16.917(スキャン#:531)
ピーク数:65 ベースピーク:173.00(19407)
スペクトル:平均 16.850-16.950(523-535)
バックグラウンド:平均 16.850-16.892(523-528)



2010/03/16 16:11:16

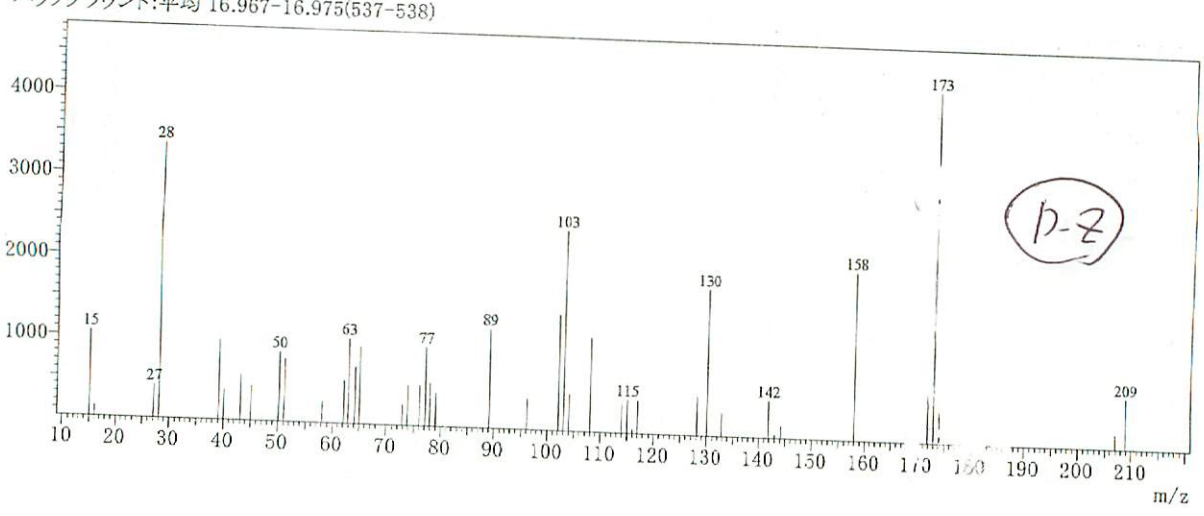
D:¥fine¥岡辺¥1129.qgd





スペクトル

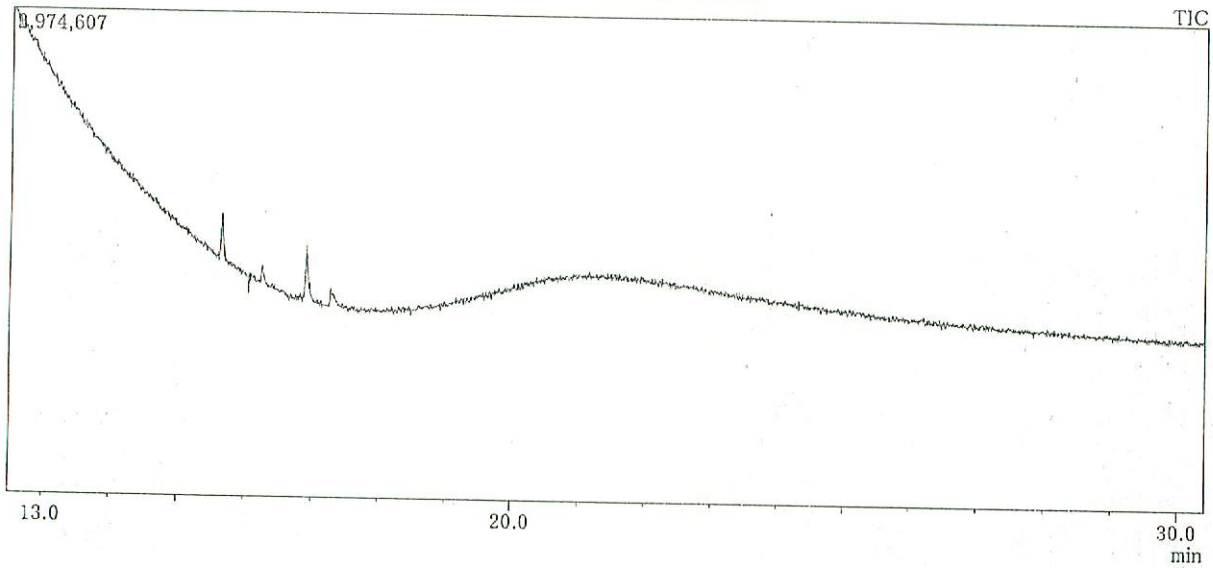
#:1 保持時間:16.958(スキャン#:536)
ピーク数:43 ベースピーク:173.00(4304)
スペクトル:平均 16.950-16.967(535-537)
バックグラウンド:平均 16.967-16.975(537-538)



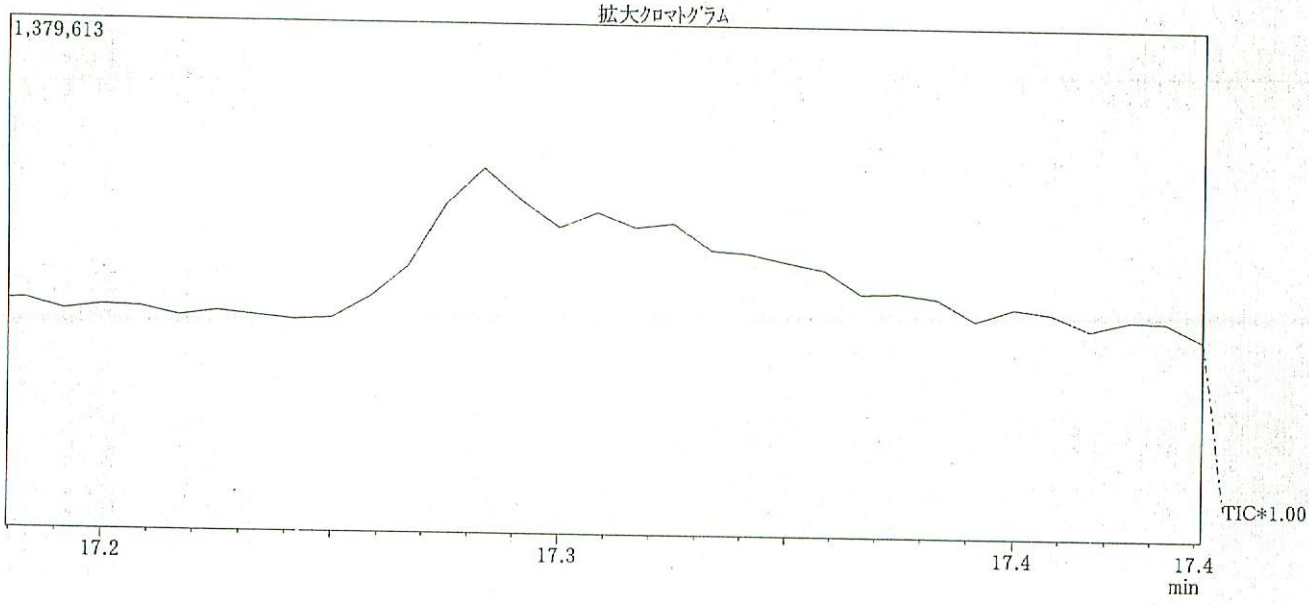
2010/03/16 10:09:42

D:¥fine¥岡辺¥1129.qgd

クロマトグラム D:¥fine¥岡辺¥1129.qgd

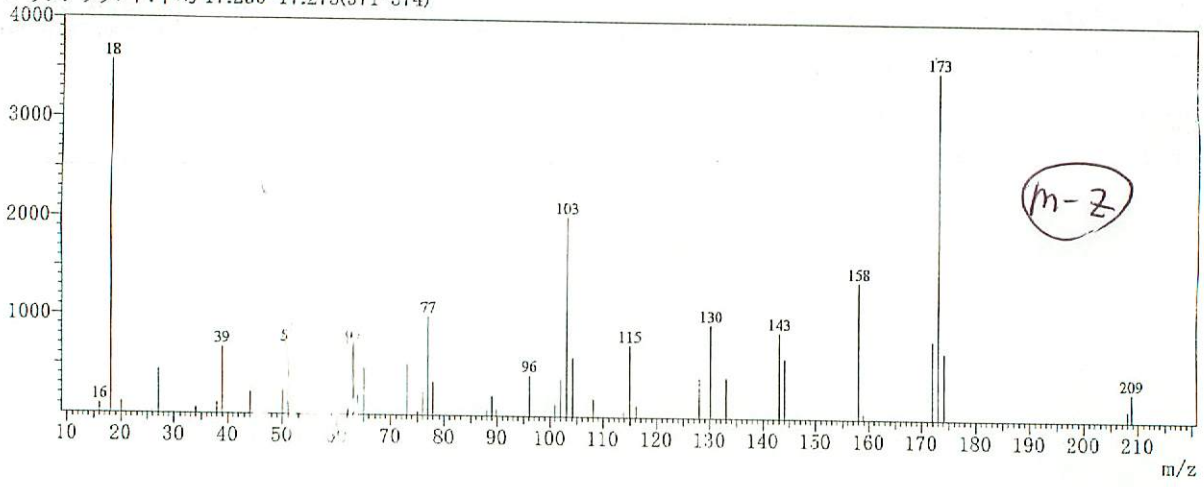


拡大クロマトグラム

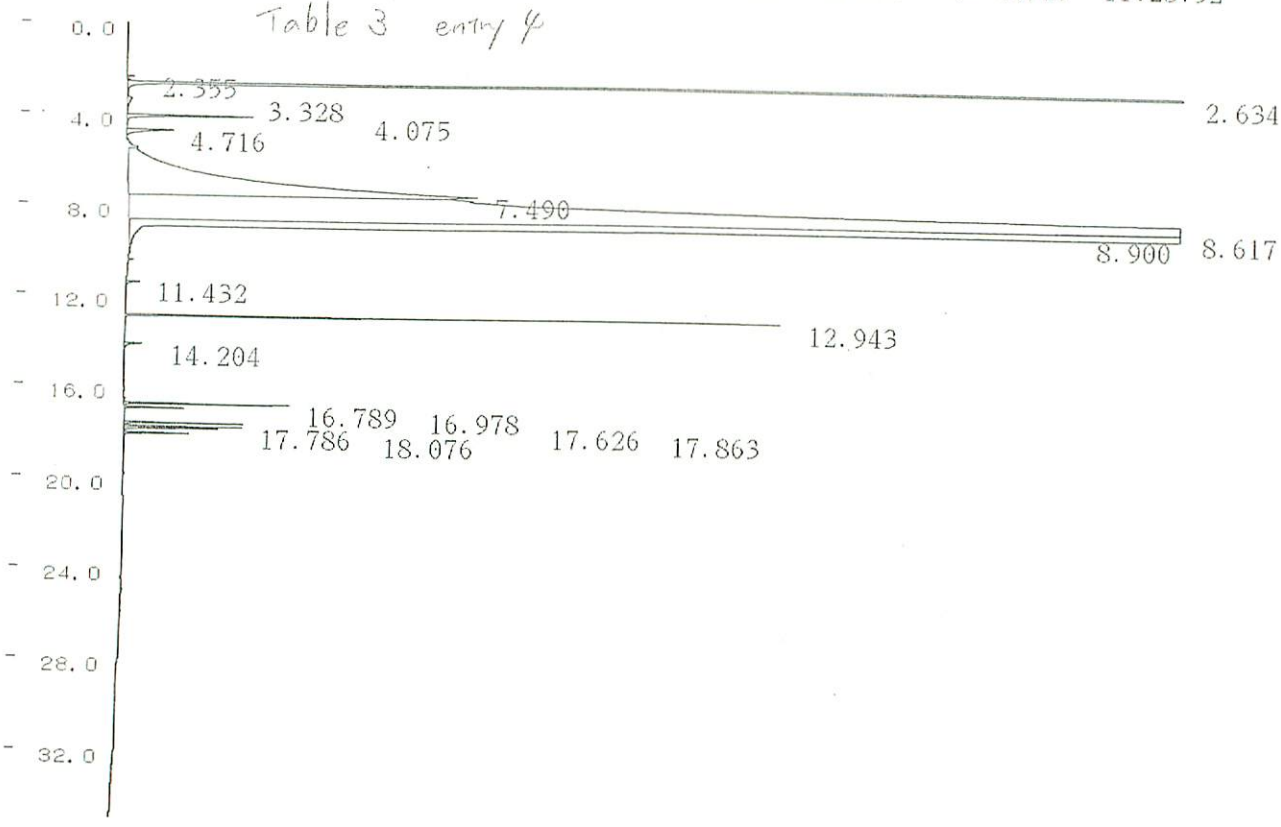


スペクトル

#:1 保持時間:17.283(スキャン#:575)
ピーク数:43 ベースピーク:18.05(3570)
スペクトル:平均 17.242-17.392(570-588)
バックグラウンド:平均 17.250-17.275(571-574)



CHROMATOPAC C-R7A CH=1 REPORT No.=4 ﾌｧｲﾙ=2:11350K.C03 00/10/15 11:28:52



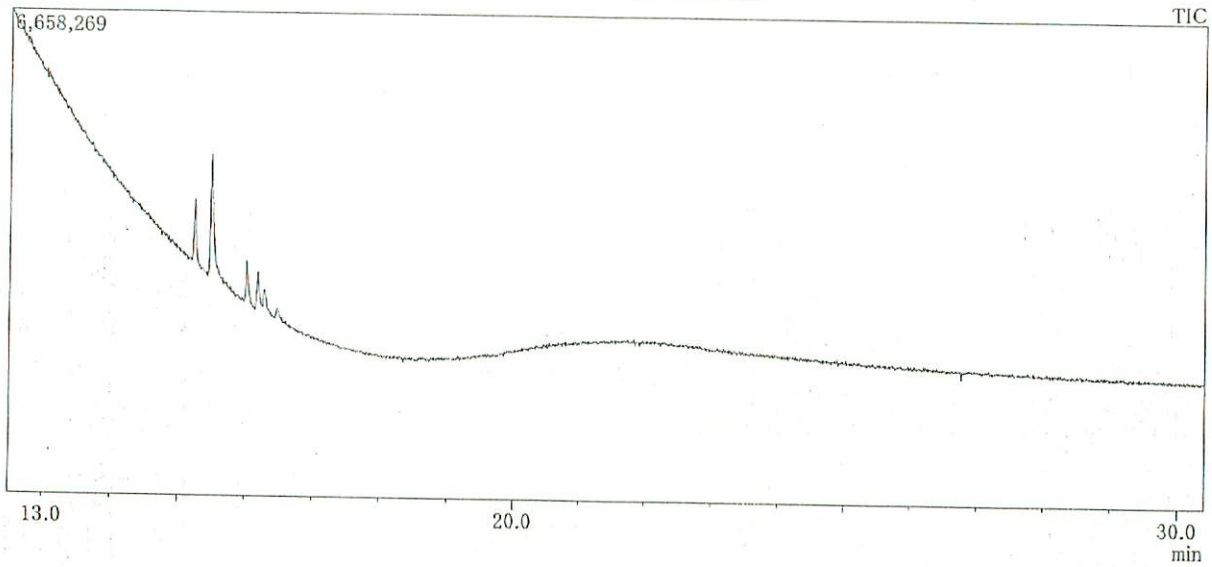
** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	1	2.355	1156	504			0.0074	
	3	2.634	2905465	1301212	V		18.562	
	4	3.328	4616	304	L		0.0295	
	6	4.075	31354	7606	L		0.2003	
	8	4.716	16925	2857	LV		0.1081	
	10	7.49	811638	20833	V		5.1853	
	11	8.617	4277458	230594	V		27.3272	
	12	8.9	7425486	838047	V		47.4389	
	15	11.432	2649	793			0.0169	
	16	12.943	85651	39538			0.5472	
	17	14.204	4625	1069			0.0295	
	22	16.789	22038	9935			0.1408	
	23	16.978	7836	3567			0.0501	
	24	17.626	16634	7147			0.1063	
	25	17.786	15967	7074	V		0.102	
	26	17.863	13332	5684	V		0.0852	
	27	18.076	9909	3924	V		0.0633	
		TOTAL	15652729	2480685			100	

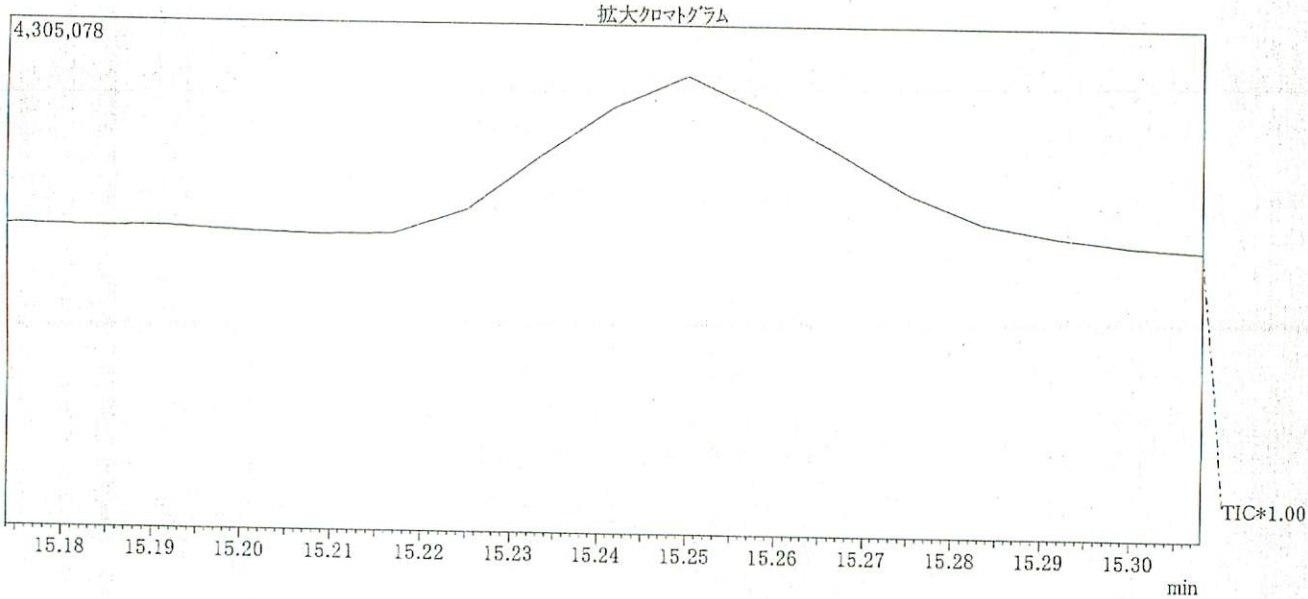
2010/03/16 10:01:10

D:¥fine¥岡辺¥1135.qgd

クロマトグラム D:¥fine¥岡辺¥1135.qgd

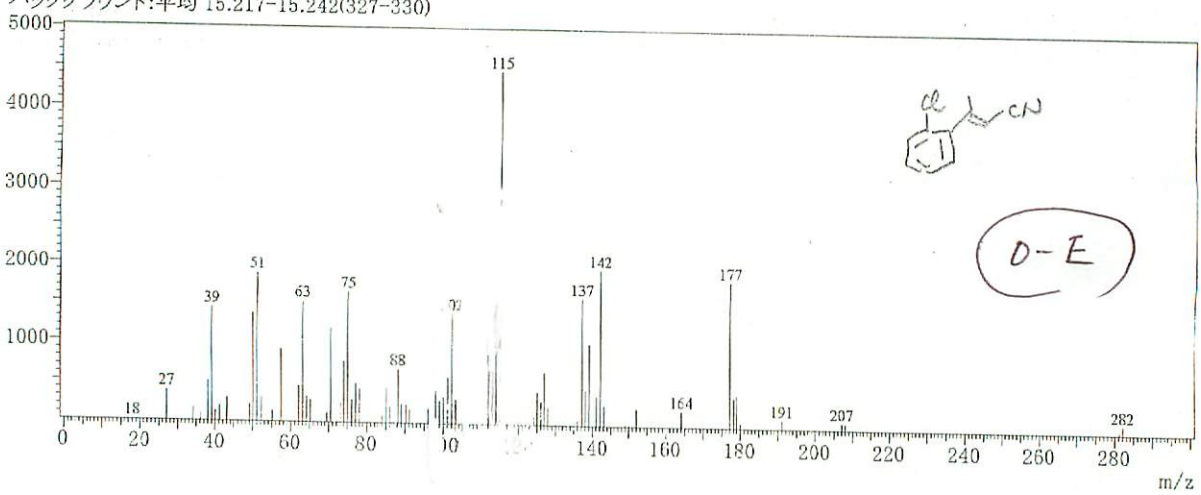


拡大クロマトグラム



スペクトル

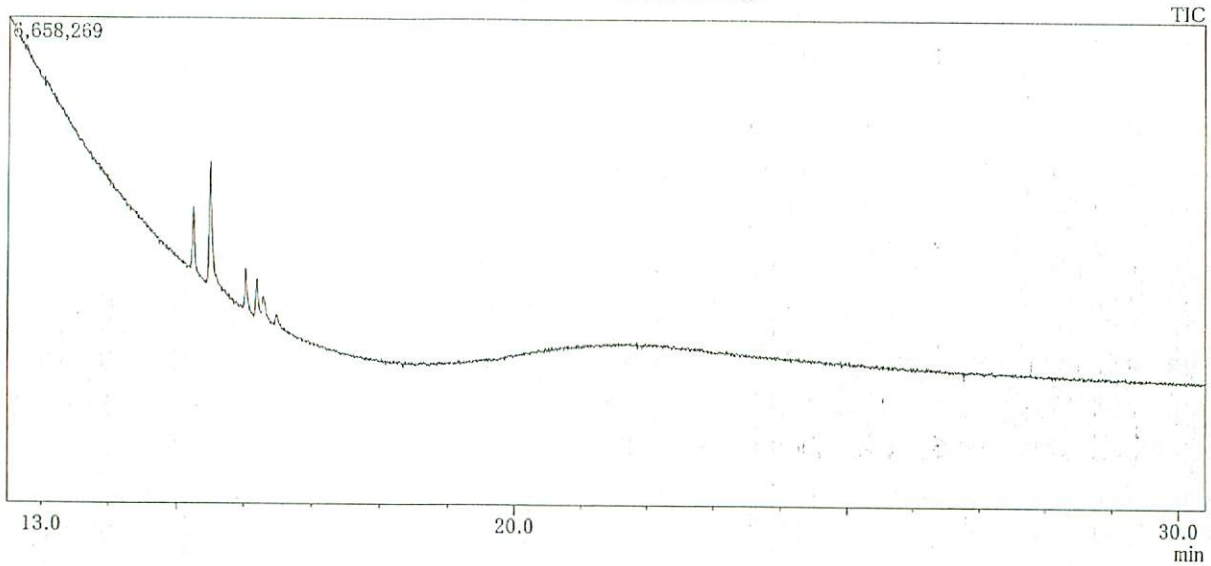
#:1 保持時間:15.250(スキャン#:331)
ピーク数:72 ベースピーク:115.10(4478)
スペクトル:平均 15.217-15.300(327-337)
バックグラウンド:平均 15.217-15.242(327-330)



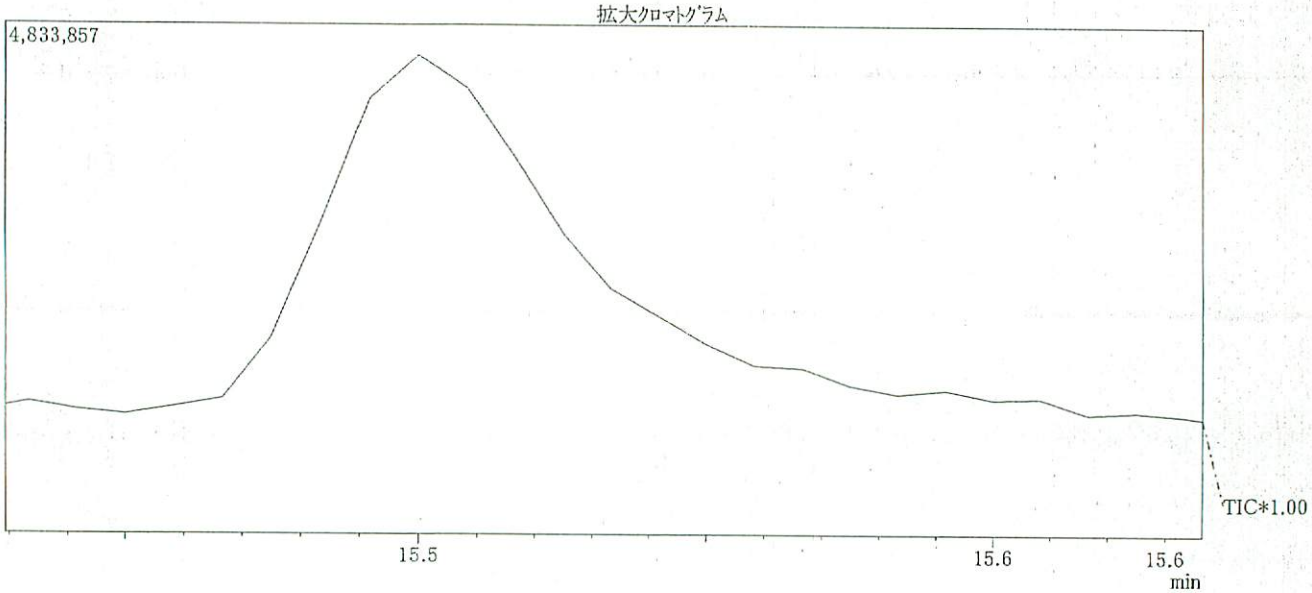
2010/03/16 13:26:48

D:¥fine¥岡辺¥1135.qgd

クロマトグラム D:¥fine¥岡辺¥1135.qgd

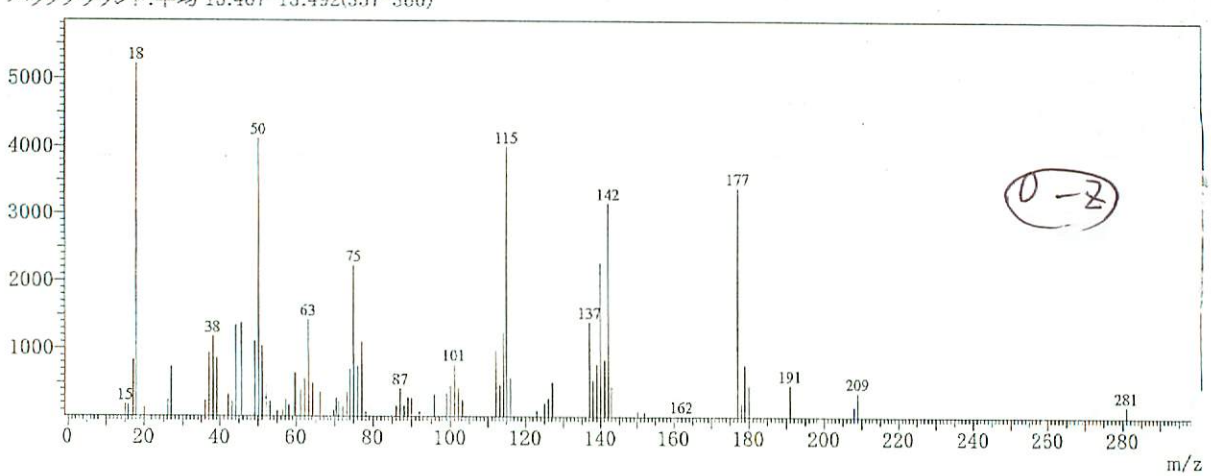


拡大クロマトグラム



スペクトル

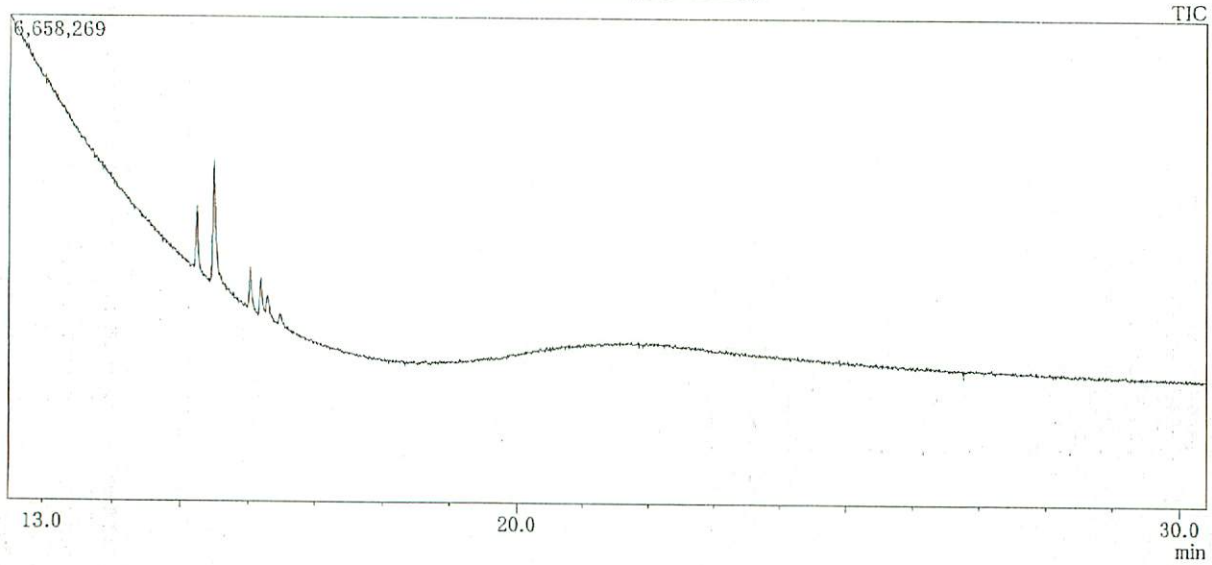
#:1 保持時間:15.500(スキャン#:361)
ピーク数:81 ベースピーク:18.05(5209)
スペクトル:平均 15.467-15.575(357-370)
バックグラウンド:平均 15.467-15.492(357-360)



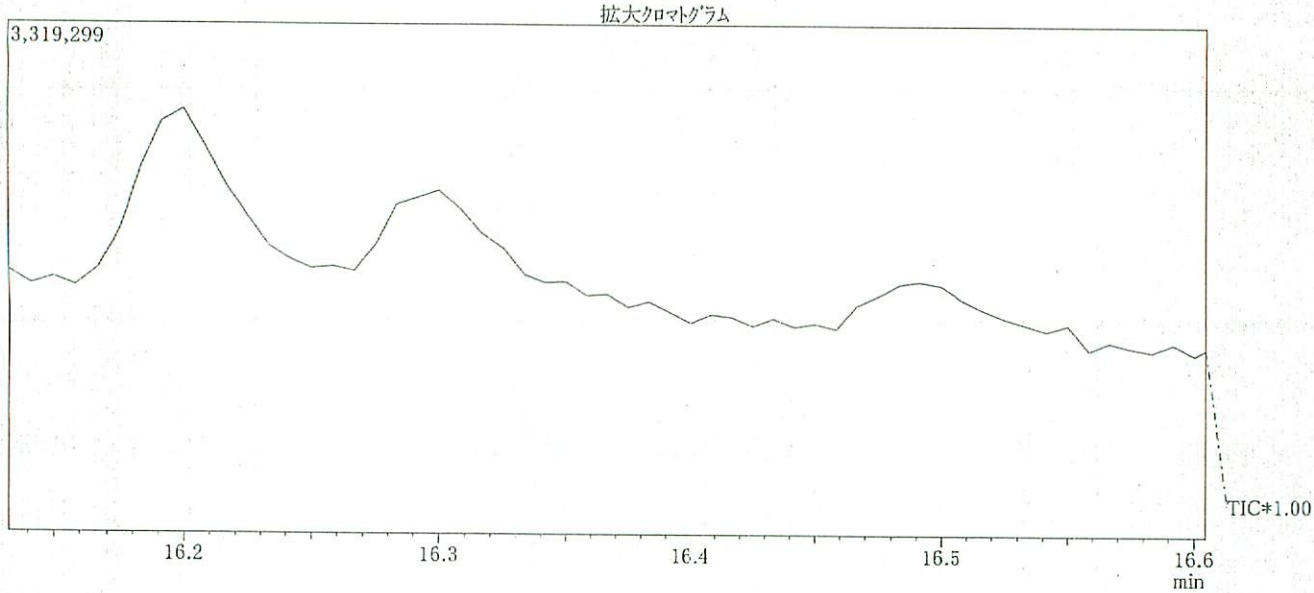
2010/03/16 13:27:59

D:¥fine¥岡辺¥1135.qgd

クロマトグラム D:¥fine¥岡辺¥1135.qgd

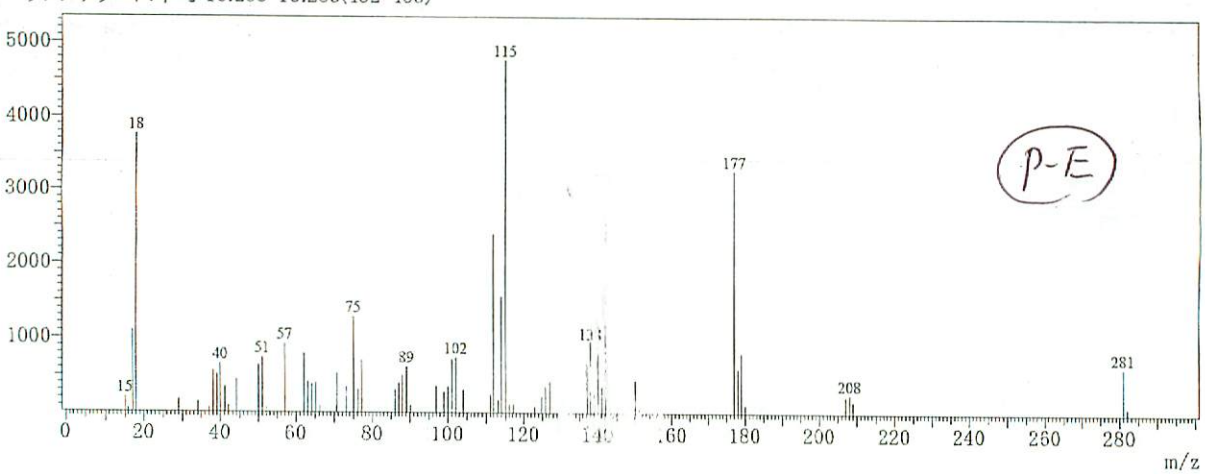


拡大クロマトグラム



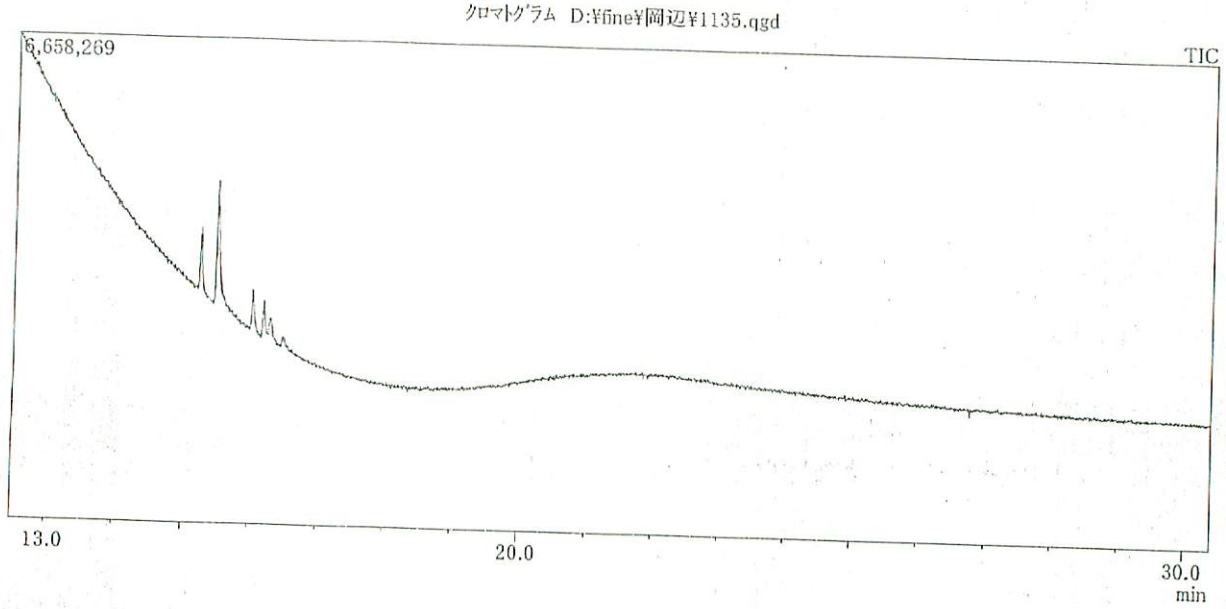
スペクトル

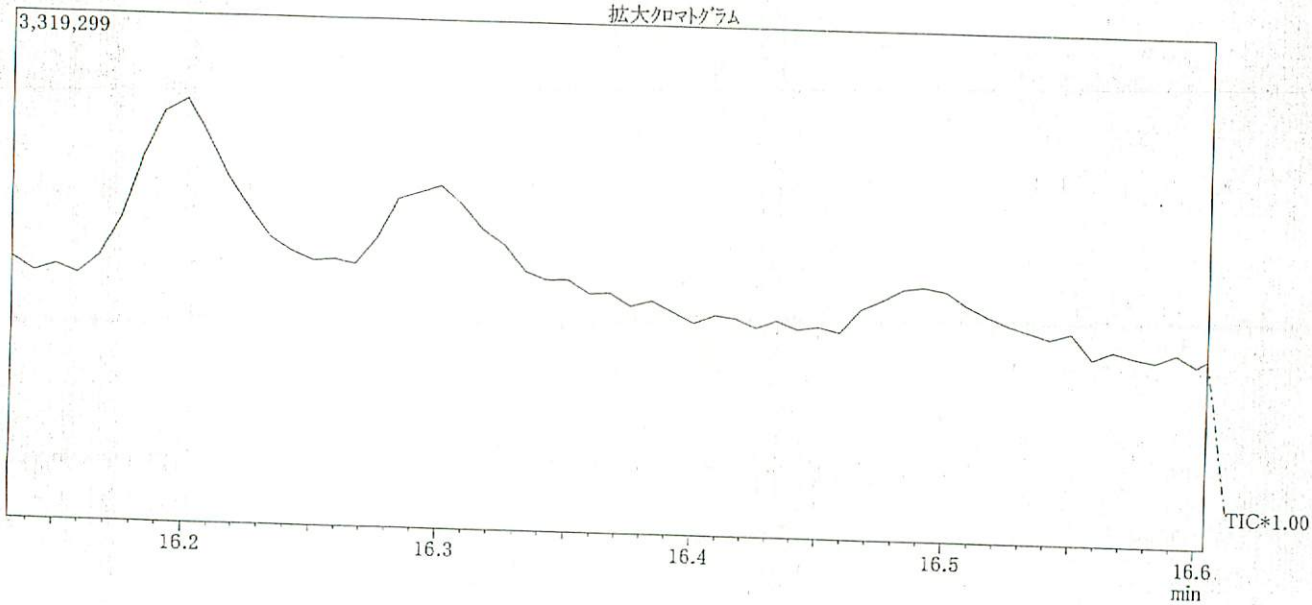
#:1 保持時間:16.300(スキャン#:457)
ピーク数:71 ベースピーク:115.10(4766)
スペクトル:平均 16.267-16.358(453-464)
バックグラウンド:平均 16.258-16.283(452-455)



2010/03/16 13:27:48

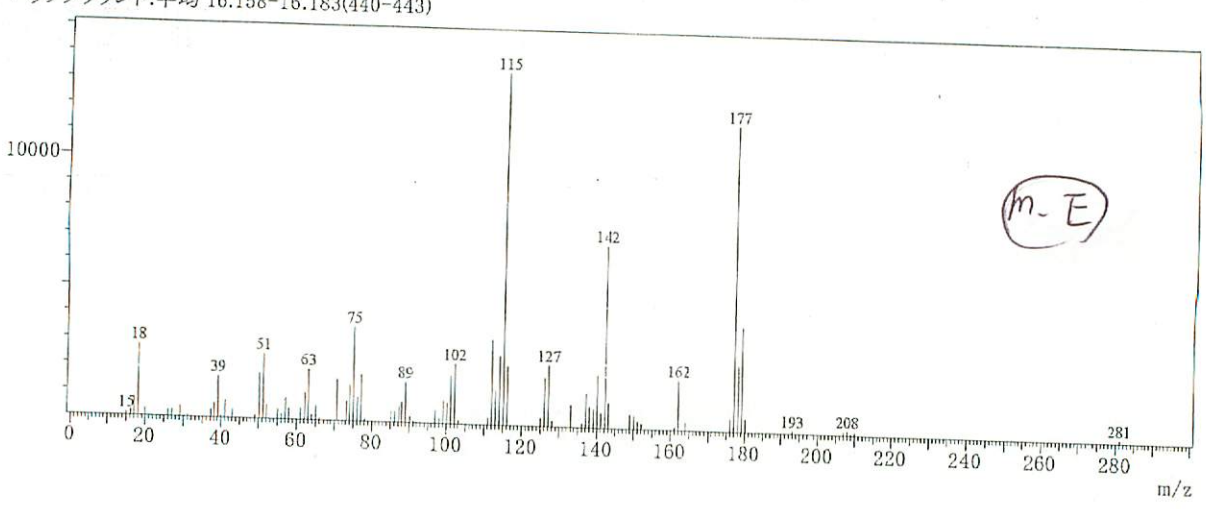
D:¥fine¥岡辺¥1135.qgd





スペクトル

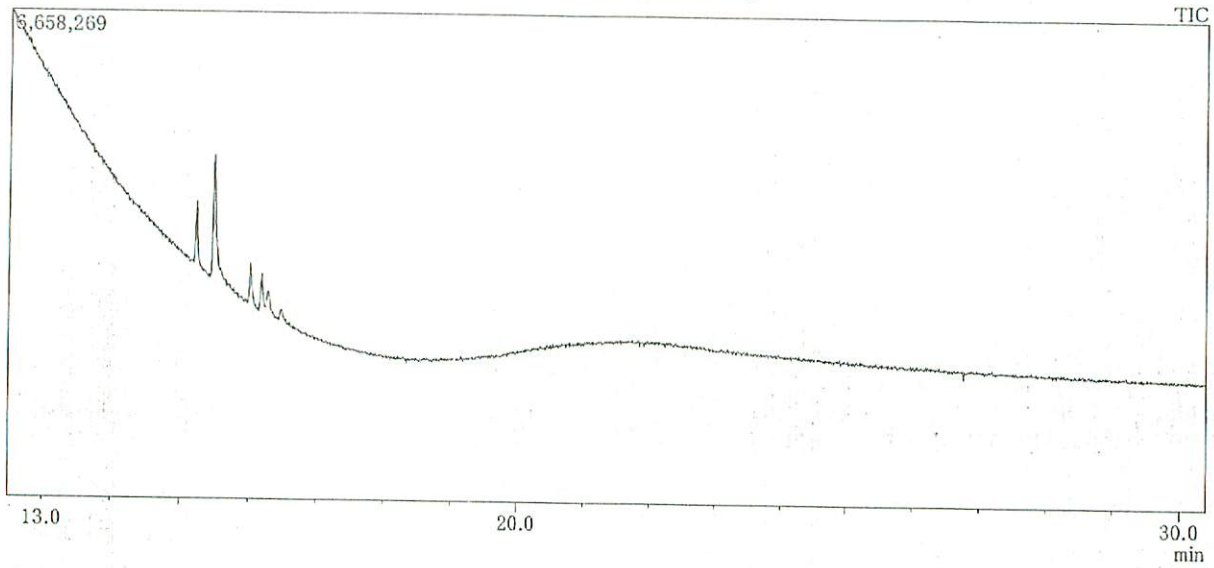
#:1 保持時間:16.200(スキャン#:445)
ピーク数:89 ベースピーク:115.10(13489)
スペクトル:平均 16.158-16.250(440-451)
バックグラウンド:平均 16.158-16.183(440-443)



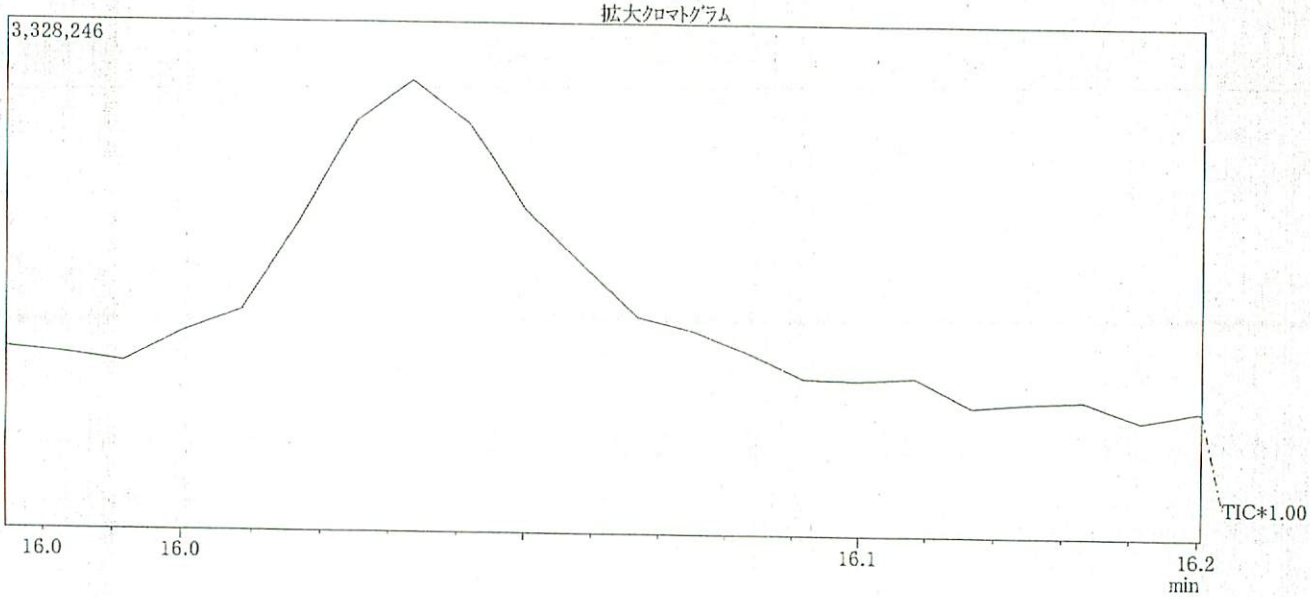
2010/03/16 13:27:31

D:¥fine¥岡辺¥1135.qgd

クロマトグラム D:¥fine¥岡辺¥1135.qgd

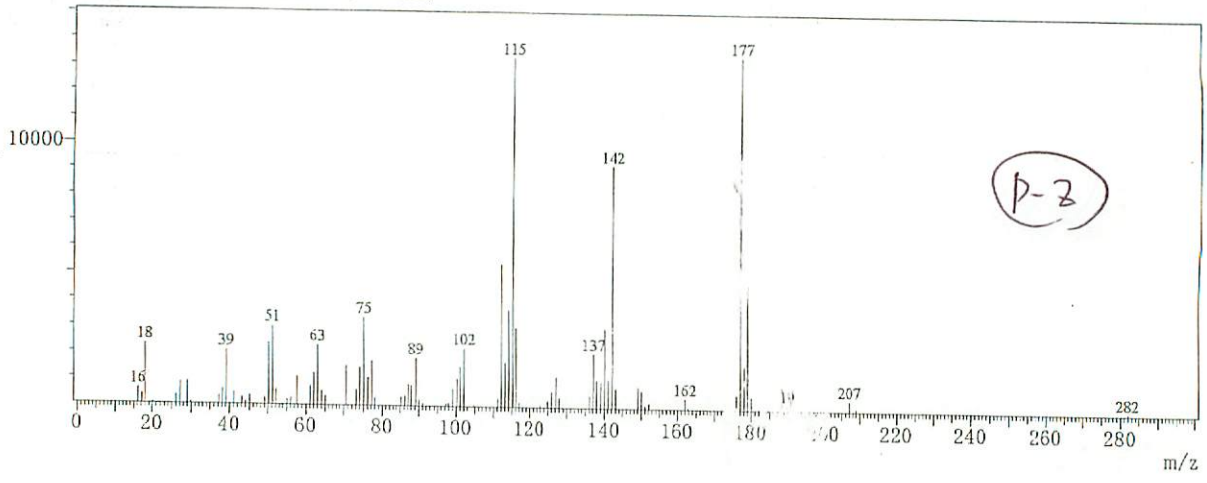


拡大クロマトグラム



スペクトル

#:1 保持時間:16.033(スキャン#:425)
ピーク数:87 ベースピーク:177.00(13443)
スペクトル:平均 15.992-16.092(420-432)
バックグラウンド:平均 15.992-16.017(420-423)

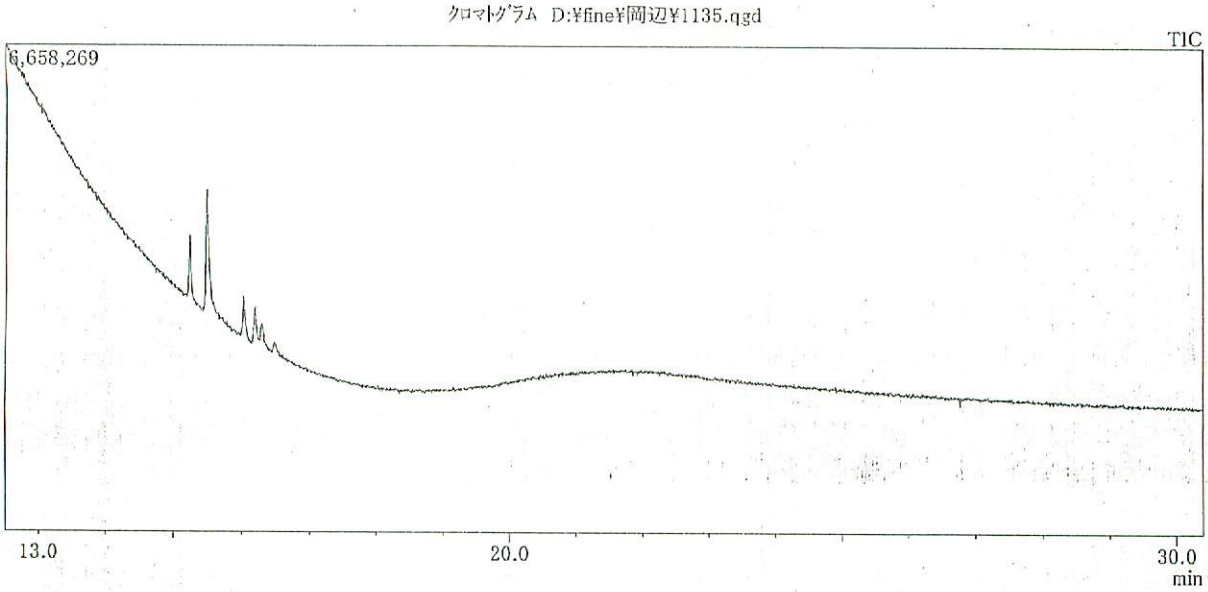


P-3

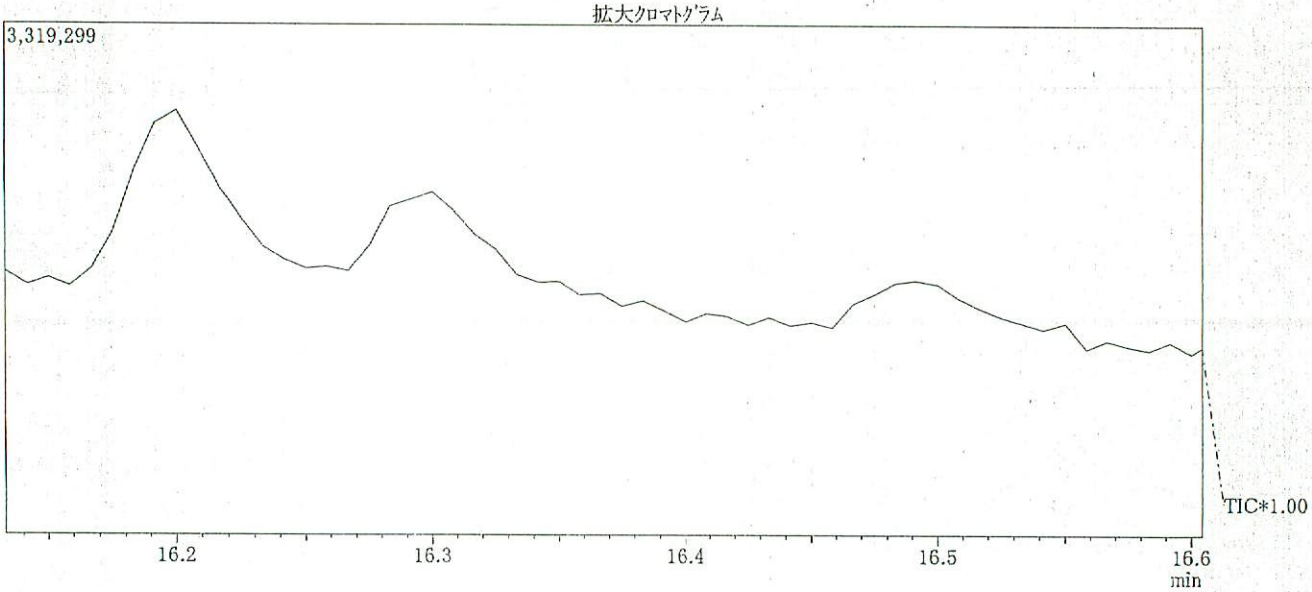
2010/03/16 13:28:15

D:¥fine¥岡辺¥1135.qgd

クロマトグラム D:¥fine¥岡辺¥1135.qgd

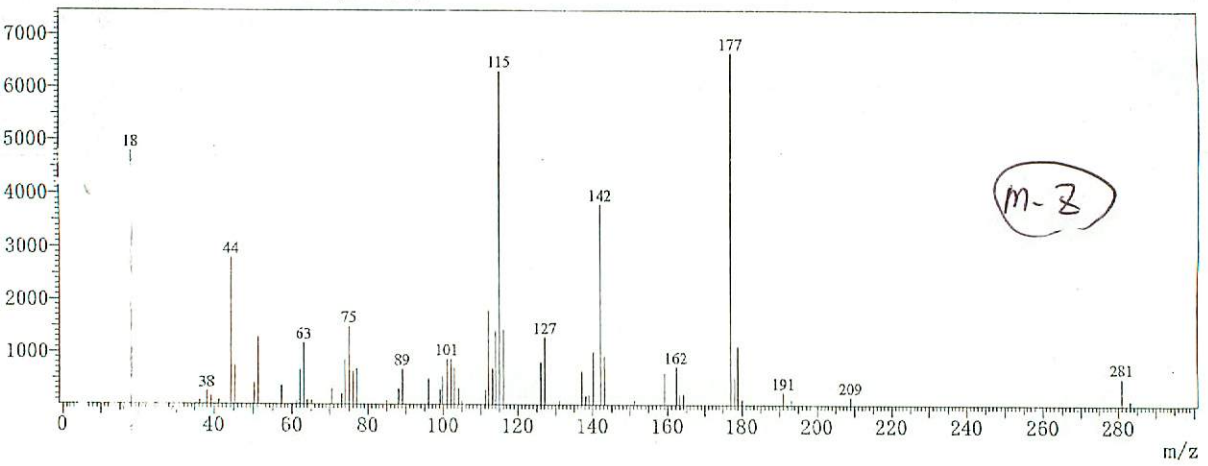


拡大クロマトグラム



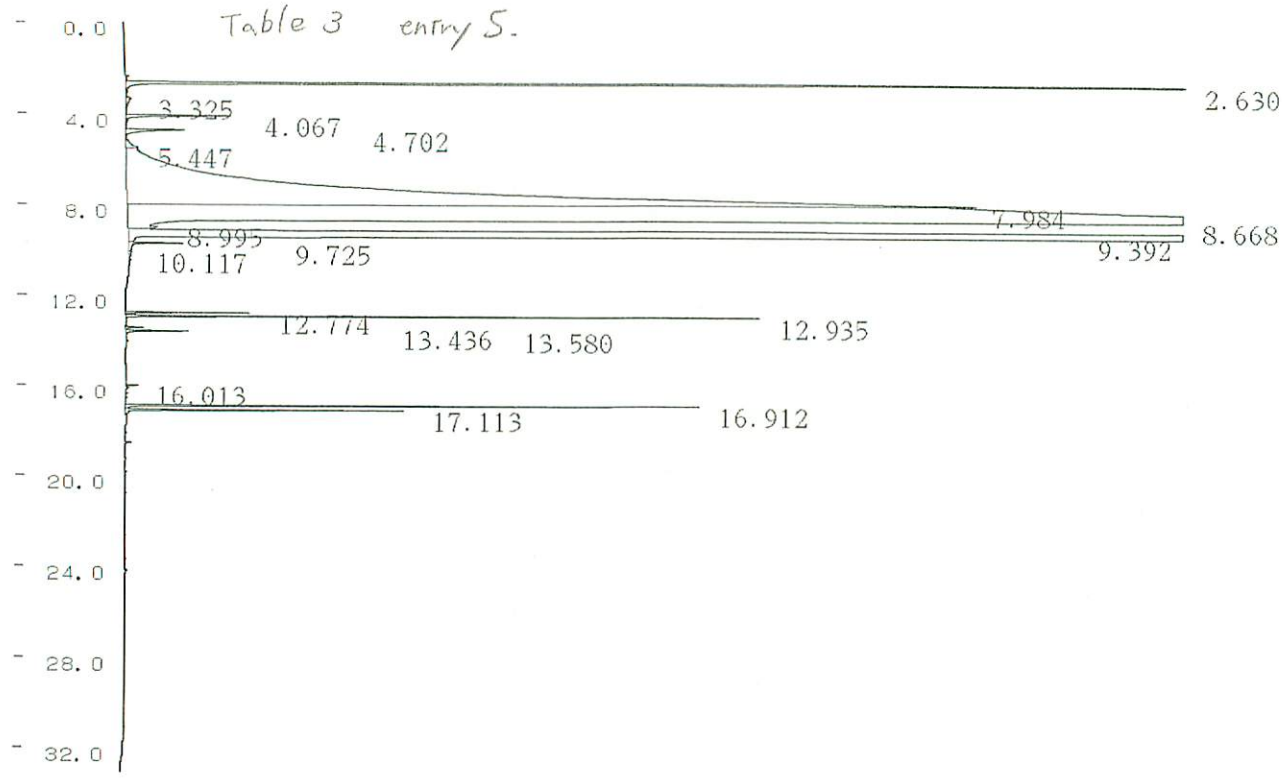
スペクトル

#:1 保持時間:16.492(スキャン#:480)
ピーク数:62 ベースピーク:177.05(6649)
スペクトル:平均 16.458-16.558(476-488)
バックグラウンド:平均 16.458-16.467(476-477)



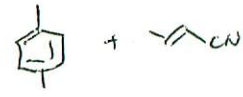
Supplementary Material (ESI) for Organic & Biomolecular Chemistry
This journal is (c) The Royal Society of Chemistry 2010

CHROMATOPAC C-R7A CH=1 REPORT No.=2 クロマト=2:1133OK.C01 C 10/15 08:54:44



** 定量計算結果 **

CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
1	3	2.63	2662938	1299330	V		15.5487	
	4	3.325	3983	285	L		0.0233	
	6	4.067	24003	6237	L		0.1402	
	8	4.702	19027	3474	L		0.1111	
	9	5.447	3726	624	V		0.0218	
	10	7.984	1848016	51156	V		10.7905	
	11	8.668	3055964	129023	SV		17.8436	
	12	8.995	1942	420	T		0.0113	
	13	9.392	9264904	1042433	V		54.0972	
	14	9.725	11458	3207	V		0.0669	
	15	10.117	1089	178	V		0.0064	
	18	12.774	15953	7406			0.0931	
	19	12.935	81570	38113	V		0.4763	
	20	13.436	3025	1075			0.0177	
	21	13.58	10248	3704	V		0.0598	
	25	16.013	1619	705			0.0095	
	30	16.912	80022	34451			0.4672	
	31	17.113	36914	16518	SV		0.2155	
	TOTAL		17126392	2638337			100	



E 8 ①

波形処理/計算エラー CH=2, 1:生ピークがありません。
CHROMATOPAC C-R7A CH=2 REPORT No.=3 クロマト=2:1134KY.C02 09/10/15 09:35:56

** 定量計算結果 ** 注意 ｴﾗｰ有 CALERROR: 1

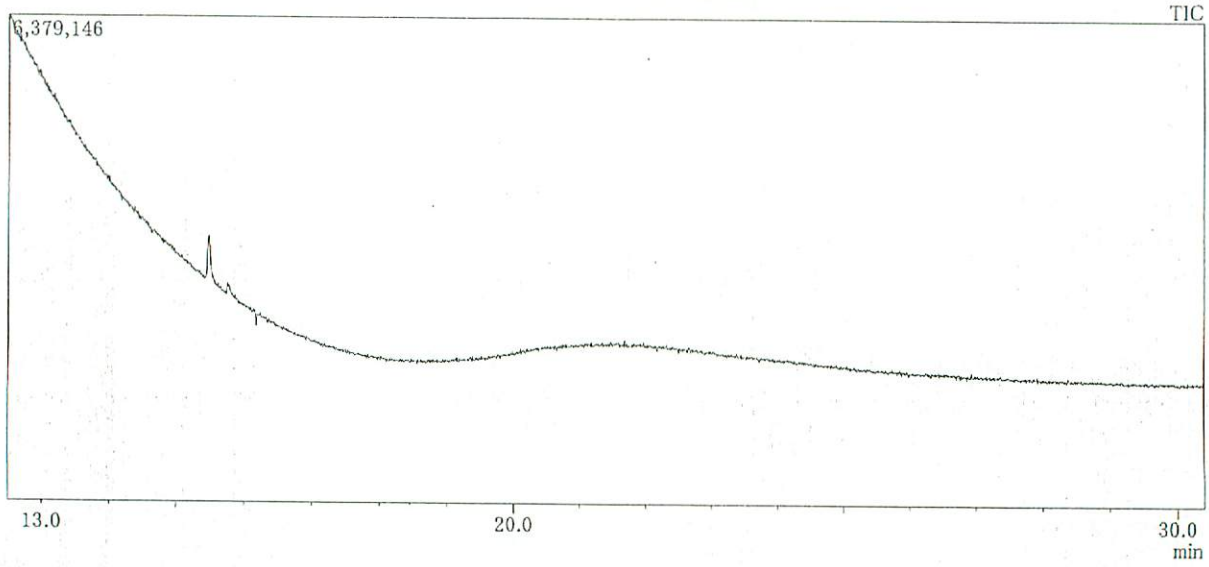
CH	PKNO	TIME	AREA	HEIGHT	MK	IDNO	CONC	NAME
	TOTAL		0	0				

1133

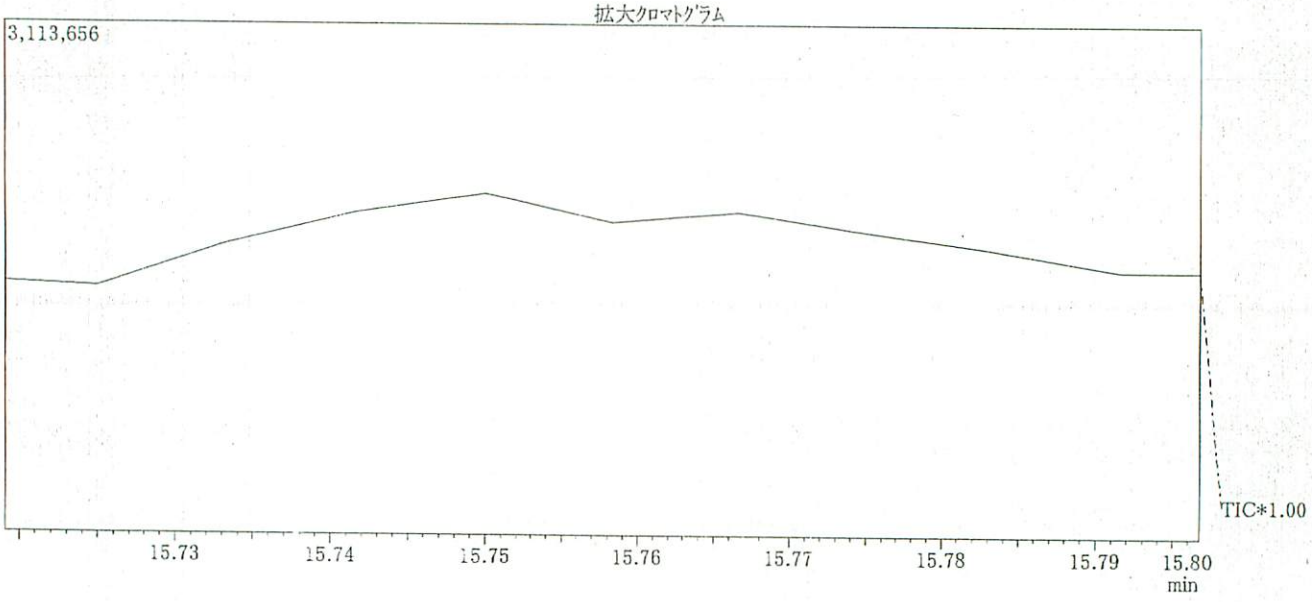
2010/03/16 10:05:32

D:¥fine¥岡辺¥1133.qgd

クロマトグラム D:¥fine¥岡辺¥1133.qgd

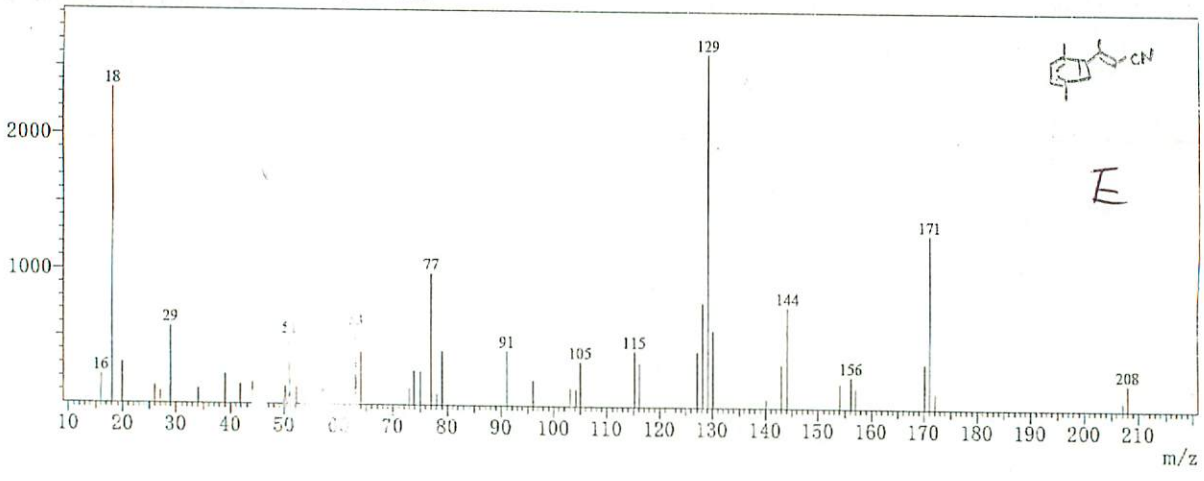


拡大クロマトグラム



スペクトル

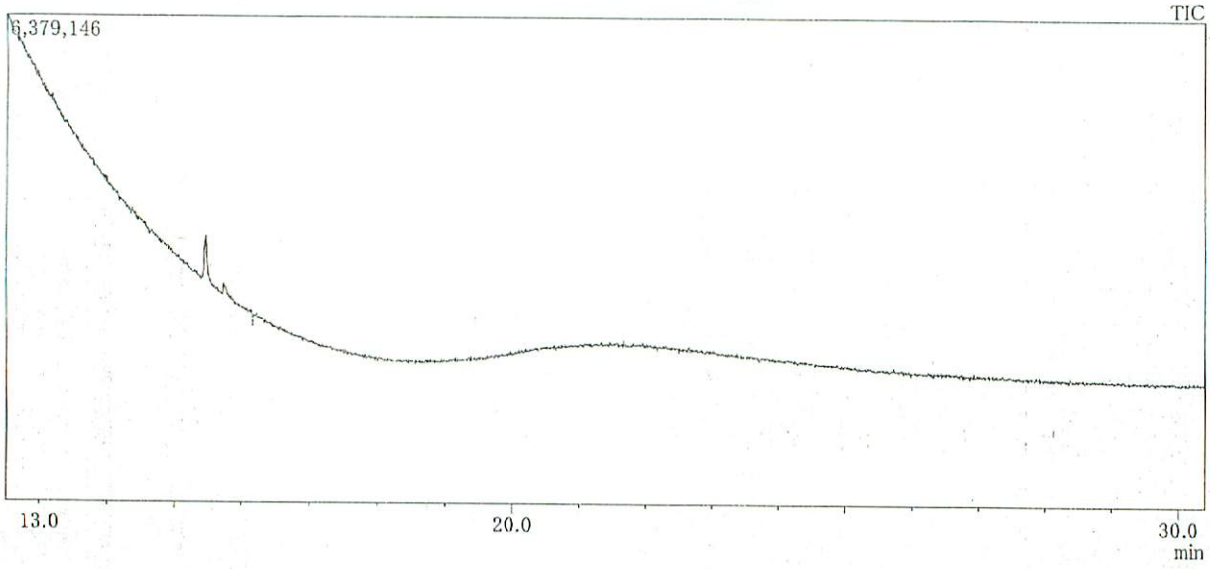
#:1 保持時間:15.750(スキャン# 391)
ピーク数:46 ベースピーク:129.10(2609)
スペクトル:平均 15.725-15.792(388-396)
バックグラウンド:平均 15.725-15.750(388-391)



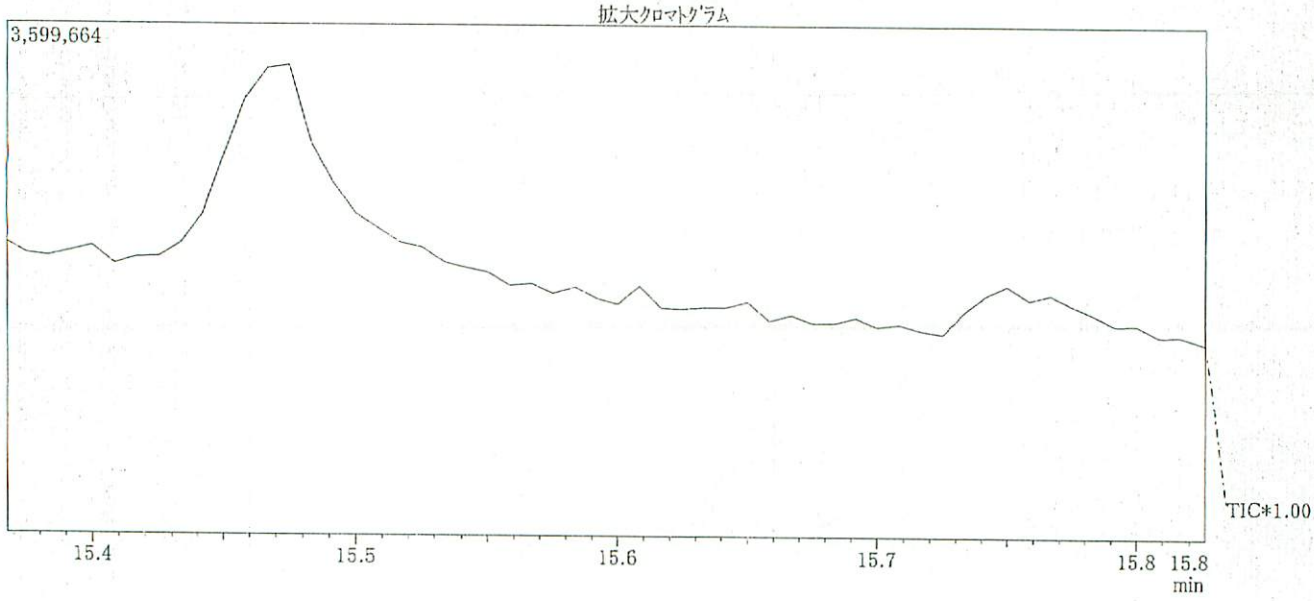
2010/03/16 10:05:04

D:¥fine¥岡辺¥1133.qgd

クロマトグラム D:¥fine¥岡辺¥1133.qgd



拡大クロマトグラム



スペクトル

#:1 保持時間:15.475(スキャン#:358)
ピーク数:80 ベースピーク:129.10(18107)
スペクトル:平均 15.425-15.525(352-364)
バックグラウンド:平均 15.417-15.458(351-356)